

# Various total cross-sections for electron impact on C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub> and CH<sub>3</sub>X (X = CH<sub>3</sub>, OH, F, NH<sub>2</sub>)

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**Abstract.** Cross-sections for the impact of electrons having energy  $E_i = 50\text{--}5000$  eV are evaluated for polyatomic molecules C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, CH<sub>3</sub>OH, CH<sub>3</sub>F and CH<sub>3</sub>NH<sub>2</sub>. Total (complete) cross-sections and total inelastic cross-sections are calculated for these targets by employing the atomic optical potentials and additivity rules. A variant of our previous work, to be called MAR–SC has been developed for molecules such as the present ones, where two approximately independent scattering centres can be identified. We find a good general accord of our theoretical values with various experimental data. Also given presently is an analytical fit  $Q_T = A (\alpha_o/E_i)^B$ , incorporating polarizability  $\alpha_o$ , for the high energy total cross-sections for 18-electron targets. Tentative upper and lower limits for the electron molecule total ionization cross-sections are identified and a break-up into elastic and inelastic contributions is exhibited.

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## 1 Introduction

There has been a sustained interest in the study of the impact of electrons on various polyatomic molecules. The intermediate and high energy domain considered presently allows for a large number of open channels, of which the rotational and vibrational channels are relatively weaker. In this region of energy ( $E_i = 50\text{--}5000$  eV) a good number of experimental investigations as compared to a few theoretical ones, have been carried out on different molecular targets. We have, uptill now, calculated various total cross-sections for the intermediate and high energy electrons scattered by simple molecules. These include CO, NO, O<sub>3</sub>, NO<sub>2</sub> *etc.* [1], H<sub>2</sub>O and 10-electron molecules [2] and also targets like [3] CH, NH, OH, H<sub>2</sub>S, OCS and SO<sub>2</sub>. The present investigation considers collisions of electrons with some of the hydrocarbons and methyl-group molecules, as mentioned in the title. In the last few years several investigations have been done on the electron scattering properties of these systems. Sueoka and Mori [4] measured total cross-sections for C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub> and C<sub>2</sub>H<sub>6</sub> in the range 1–400 eV. At these energies, scattering experiments on various hydrocarbons were also performed by Floeder *et al.* [5] and by Nishimura and Tawara [6]. Recently, Szymtkowski and Krzysztofowicz [7] have measured total cross-sections for CH<sub>3</sub>X (X = CH<sub>3</sub>, OH, F, NH<sub>2</sub>) targets upto 250 eV energy. Several experimental groups *e.g.*, Zheng and Srivastava [8], Chatham *et al.* [9] have reported total ionization cross-sections from threshold upwards, for

some of these molecules, while Hwang *et al.* [10] have calculated the theoretical ionization cross-sections for various molecules, in the Binary Encounter Bethe model. Jain and Baluja [11] constructed complex optical potentials based on molecular wave functions and charge densities and calculated total cross-sections for a variety of molecules including C<sub>2</sub>H<sub>2</sub>. Jiang *et al.* [12] calculated total cross-sections for C<sub>2</sub>H<sub>4</sub> and other molecules, on the basis of a simple “Additivity rule” that was used by us earlier. These authors have recently [13] given energy-dependent geometrical additivity rule (EGAR). However, they could not employ molecular properties like bondlength and polarizability explicitly.

The additivity rules in the simple and modified form [1–3] offer reasonable approximations to  $e^-$ -molecule total cross-sections at high enough energies beyond 100 eV. The total inelastic cross-sections calculated by us in these approximations also offer a reliable theoretical high energy limit to the total ionization cross-sections, for various  $e^-$ -molecule systems. Further for molecules containing H-atom(s), we employed [3] the single-centre expansions to derive reliable theoretical cross-sections. Now, our aim in this paper is to employ all these approximations to obtain theoretical cross-sections for the present list of molecules, for which previous theoretical data are scarce. In view of the nature of these molecules we have now developed a realistic additivity approximation based on groups of atoms, rather than individual atoms. About three decades back, Schram *et al.* [14] measured gross total ionization cross-sections of various

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**Table 1.** Properties of target molecules<sup>(a)</sup>.

Molecule (No. of electrons)	Bond length <sup>(a)</sup> ( $a_o$ )	Dipole moment (a.u.)	Ionization energy (eV)	Average polarizability ( $\alpha_o a_o^3$ )
C <sub>2</sub> H <sub>2</sub> (14)	C–H 2.04	0	11.41	24.51
	C–C 2.05			
C <sub>2</sub> H <sub>4</sub> (16)	C–H 2.05	0	10.50	28.72
	C–C 2.51			
Ar (18)	–	0	15.76	11.11
H <sub>2</sub> S (18)	S–H 2.54	0.38	10.41	26.68
C <sub>2</sub> H <sub>6</sub> (18)	C–H 2.09	0	11.50	30.19
	C–C 2.90			
CH <sub>3</sub> OH (18)	C–H 2.07	0.67	10.84	22.22
	C–O 2.69			
	O–H 1.81			
CH <sub>3</sub> F (18)	C–H 2.07	0.73	12.85	20.06
	C–F 2.61			
CH <sub>3</sub> NH <sub>2</sub> (18)	C–H 2.06	0.73	11.73	27.09
	C–N 2.78			
	N–H 1.91			

<sup>(a)</sup> See Lide [15] (CRC handbook of Physics and Chemistry).

hydrocarbon molecules. They used the additivity concept to express this cross-section as a sum of contributions from various chemical bonds in alkanes and alkenes, at high impact energies. Presently we have also clarified in brief the underlying theoretical picture.

Important properties [15] of our target molecules, have been shown through Table 1, as an aid to clarify the method and the approximations involved in the present calculations.

## 2 Theory and calculations

In a high energy approximation, we consider spherical interactions only and express the  $e^-$ -molecule total (elastic + inelastic) cross-section  $Q_T(M)$  in a simple additivity rule – AR [1–3] as follows

$$Q_T(M) = \sum_{i=1}^n Q_T^{(i)}(A). \quad (1)$$

where the RHS is a sum of the total cross-sections for all the  $n$  atoms of the molecule. The free-atom cross-section  $Q_T^{(i)}(A)$  is calculated in a complex optical potential approach such that for the  $i$ th atom,

$$Q_T^{(i)} = Q_{el}^{(i)} + Q_{inel}^{(i)} \quad (2)$$

with the two terms on the RHS representing total elastic cross-section and the total inelastic cross-section respectively for atom  $i$ . As discussed earlier [3] the molecular total inelastic cross-section  $Q_{inel}$  itself can also be

expressed as sum of atomic inelastic cross-sections in this approximation. Thus,

$$Q_{inel}(M) = \sum_{i=1}^n Q_{inel}^{(i)}(A). \quad (3)$$

The total molecular inelastic cross-section  $Q_{inel}$  is the theoretical upper limit of the electron impact ionization cross-section  $Q_{Ion}(M)$ . From equation (3)  $Q_{inel}(M)$  is calculated through the atomic total inelastic cross-sections  $Q_{inel}^{(i)}(A)$ . The latter quantity is calculated by defining an electron-atom absorption potential  $V_{abs}(r, E_i)$  which is given in a Pauli-blocking local form in reference [16]. This absorption potential [16] depends on the charge-density and electronic excitation energy (or ionization energy) of the target, and the incident energy of the projectile. Jain and Baluja [11] had employed the same absorption model, but they used a direct molecular charge-density as an input to express  $V_{abs}$  therein. In general  $Q_{inel}(M)$  includes the effect of ionization as well as electronic excitations, but with the increase of impact energy, the ionization dominates all the inelastic processes. Hence the  $Q_{inel}$  is comparable with calculated or measured  $Q_{Ion}$ . From equation (3) the additivity rule [1–3, 17] for molecular total ionization cross-section  $Q_{Ion}(M)$  follows as given here under

$$Q_{Ion}(M) = \sum_{i=1}^n Q_{Ion}^{(i)}(A) \quad (4)$$

where RHS is the sum of the relevant  $e^-$ -atom ionization cross-sections. Now, equations (1, 3, 4) are rather too simple, in that they do not employ any molecular property. Previously [1–3] we introduced a correction in the AR,

equation (1), by considering the long-range  $e^-$ -*molecule* polarization interaction explicitly. The simple addition vide equation (1) is now restricted to short-range (static, exchange and absorption) potentials in our Modified Additivity Rule-MAR, [1–3] *viz.*,

$$Q_T(M) = \sum_{i=1}^n Q_{SR}^{(i)} + Q_{pol}(M) \quad (5)$$

where, the first term on the RHS is the sum of  $e^-$ -*atom* cross-sections calculated in the short-range complex potential, and the second term represents the total cross-section due to the direct  $e^-$ -*molecule* polarization potential separately.  $Q_{pol}(M)$  is calculated by employing molecular polarizability (Tab. 1) and it offers a small contribution which rapidly decreases with  $E_i$ . The cross-sections  $Q_{SR}^{(i)}$  are calculated by treating the complex short-range atomic optical potential exactly in the partial wave analysis. This complex potential incorporates the static, exchange and absorption terms. The standard formalism for calculating the cross-section is given in [18]. The  $e^-$ -*molecule* polarization effect is treated similarly by employing an energy-dependent model potential well-known in literature. The AR (Eq. (1)) and the MAR (Eq. (5)) merge for high energy scattering dominated by static and absorption potentials. When  $E_i$  exceeds about 300 eV, the molecular total cross-section  $Q_T(M)$  is a sum of elastic and inelastic (mainly ionization) cross-sections.

In our earlier calculations on HF, OH, NH, CH and also H<sub>2</sub>S (see Ref. [3]) use was also made of a formulation based on single-centre expansions, involving [19] the Bessel functions. We expanded the charge-density of the H-atom(s) in the target molecule, at the nucleus of the heavier (partner) atom. The resulting single-centre (SC) molecular charge-density was employed to construct the full  $e^-$ -*molecule* spherical complex potential and to calculate the cross-sections. This approximate calculation [3] is realistic in that, it employs actual molecular properties like bondlength(s), ionization energy and polarizability. Our results agree better than those derived [11] with molecular wave functions and charge-densities.

Now, keeping in view the target molecules of our present work, let us introduce a further modification by combining suitably the MAR and the SC approaches mentioned above. Each of the molecules C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub> and C<sub>2</sub>H<sub>6</sub> exhibits a smaller C–H bondlength and a larger C–C bondlength. In passing from C<sub>2</sub>H<sub>2</sub> to C<sub>2</sub>H<sub>6</sub>, the C–C bondlength actually increases. Thus at high energy (and the short wavelength) of the incident electron, the two carbon atoms in these molecules serve as approximately independent scattering centres. The contributions from Hydrogen atoms in the C–H bonds can be considered through the single-centre expansions. We, therefore, expand the H-atom charge-density  $\rho_H$  at the C-atom of each C–H bond in the molecule. Hence, the spherical SC charge-density of a typical CH<sub>*n*</sub> group, labeled as  $\rho_G$ , takes the form:

$$\rho_G(r, R_{C-H}) = \rho_C(r) + n\rho_H(r, R_{C-H}) \quad (6)$$

where,  $r$  is the radial distance from the carbon nucleus and the bond-lengths  $R_{C-H}$  are already tabulated. The molecule is represented here by TWO groups of atoms rather than by individual atoms. The number of H-atoms at each C-atom is,  $n = 1, 2$  and  $3$  for C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub> and C<sub>2</sub>H<sub>6</sub> respectively. The SC charge-density per scattering centre normalizes to 7 (half of the total 14) electrons in C<sub>2</sub>H<sub>2</sub>, 8 electrons in C<sub>2</sub>H<sub>4</sub> and 9 electrons in C<sub>2</sub>H<sub>6</sub>. Equation (6) can be further improved if the bond-charges acquired by the partner atoms during the formation of covalent bonds are known [20].

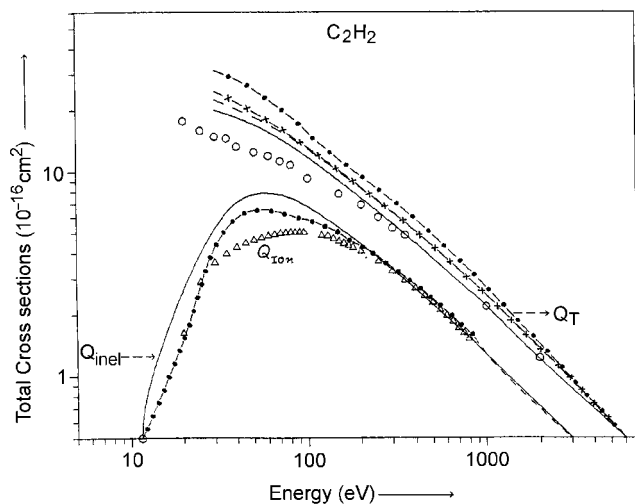
Further for the 18-electron CH<sub>3</sub>X molecules, we again identify two scattering centres, *viz.* one at the C-atom and the other at the heavier atom in of the X (= CH<sub>3</sub>, OH, F, NH<sub>2</sub>) group. At each scattering centre, the SC charge density (of Eq. (6)) is normalized to 9 electrons as required. Next, the said single centre charge density is employed to construct a short-range complex optical potential incorporating static, exchange and absorption terms, based on the well-known models [1]. It is thus possible to calculate a short-range contribution  $Q_{SR}(\alpha)$  from each scattering centre  $\alpha$  ( $= 1, 2$ ) to the total  $e^-$ -*molecule* (elastic + inelastic) cross-section  $Q_T(M)$ . Finally we combine the MAR of equation (5) with this SC approach to write,

$$Q_T(M) = \sum_{\alpha=1}^2 Q_{SR}(\alpha) + Q_{pol}(M). \quad (7)$$

In equation (7)  $Q_{pol}(M)$  is calculated by defining the  $e^-$ -*molecule* polarization potential as a function of distance  $r_o$  from the molecular centre of mass. The  $Q_{SR}(\alpha)$  corresponding to each scattering centre  $\alpha$  is obtained through SC charge-density as explained. In the case of CH<sub>3</sub>F molecule, we define one of the scattering centres at C, the other being the F atom itself. The separations between the two scattering centres (*e.g.* C–C bondlength) are large enough to justify the modified additivity rule with single centre expansion (MAR–SC), equation (7) at high energies. Moreover, it offers a convenient, simple and effective method for these polyatomic molecules. Presently it is also possible to calculate the inelastic TCS  $Q_{inel}$  for these molecules. Recognizing the two scattering centres as stated above, we obtain the SC charge density at each of them. We then construct the absorption potential [16] to calculate  $Q_{inel}(\alpha)$  for each of them. Thus the total molecular  $Q_{inel}$  is the sum of the cross-sections from the two centres *i.e.*

$$Q_{inel}(M) = \sum_{\alpha=1}^2 Q_{inel}(\alpha). \quad (8)$$

Again this approach is better than a simple atomic addition vide equation (3). Schram *et al.* [14] partitioned the molecular  $Q_{Ion}(M)$  into contributions arising from different chemical bonds in the target molecule. They did not provide any theoretical background for such an additivity rule. Considering CH<sub>4</sub> molecule as an example, the total quantity  $Q_{Ion}(M)$  can be regarded as arising mainly



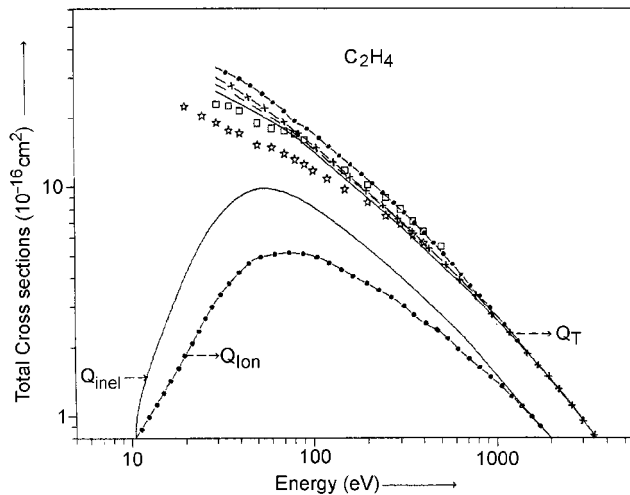
**Fig. 1.**  $e^-$ - $C_2H_2$  scattering: upper curves ( $Q_T$ ) theory: (-●-●-) Jain and Baluja [11], (-x-x-x-) AR (Eq. (1)), (- - -) MAR (Eq. (5)), (—) MAR-SC (Eq. (7)), (○ ○ ○) measurements of Sueoka and Mori [4]; lower curves theory: (—) present  $Q_{inel}$  (Eq. (8)), (-●-●-) Jain and Baluja [11], (Δ Δ Δ)  $Q_{Ion}$  measurements of Zheng and Srivastava [8].

due to the four identical C-H bonds *i.e.* all valence electrons, by neglecting the K-shell ionization in the C-atom. Schram *et al.* [14] thus estimated the partial cross-sections for a C-H bond from their experimental data on  $CH_4$  molecule, and employed the same value to various alkanes and alkenes to estimate the partial contribution of a  $\sigma(C-C)$  or a  $\pi(C-C)$  bond. In our theoretical method, we use a reasonable approximation to calculate the partial contribution of all bonds as well as core electrons associated with a scattering centre, *e.g.* a C-atom in  $C_2H_6$ . Our method *vide* equations (6, 8) takes care of the fact that the same bond may have slightly different bond-lengths in different molecules (Tab. 1).

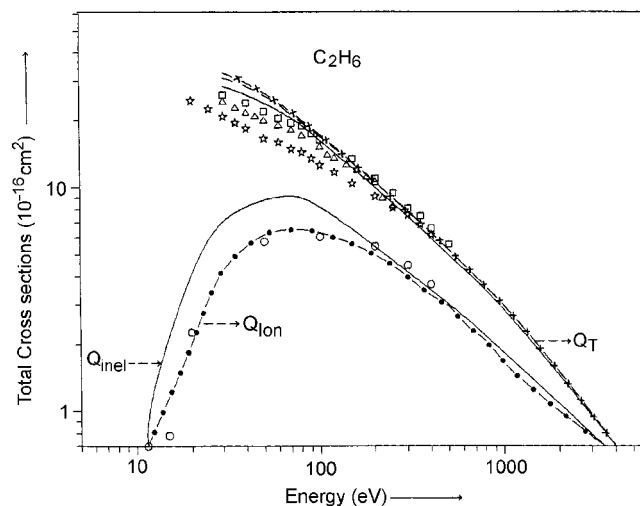
Finally one can consider a small contribution arising out of nonspherical effects, especially in polar molecules, (Tab. 1). This contribution is significant below about 100 eV. It is in this region of energy that the present approximations give overestimated results, even without the nonspherical contributions. We have, therefore, not included dipole and other nonspherical terms in the present calculations.

### 3 Results and discussion

The present paper reports the complete TCS  $Q_T(M)$  and the inelastic TCS  $Q_{inel}(M)$  for the impact of electrons on  $C_2H_2$ ,  $C_2H_4$ ,  $C_2H_6$ ,  $CH_3OH$ ,  $CH_3F$  and  $CH_3NH_2$  molecules. Our theoretical values based on various approximations discussed above, are compared with results obtained previously by other workers and are shown graphically in the Figures 1–6. The AR (Eq. (1)) does not incorporate molecular properties, and ignores multiple in-



**Fig. 2.**  $e^-$ - $C_2H_4$  scattering: upper curves ( $Q_T$ ) theory (-●-●-) Jiang *et al.* [12], (-x-x-x-) AR (Eq. (1)), (---) MAR (Eq. (5)), (—) MAR-SC (Eq. (7)), Measurements (□ □ □) reference [6], (☆☆☆) reference [4]; lower curves: (—) present  $Q_{inel}$  (Eq. (8)), (-●-●-) theoretical  $Q_{Ion}$  reference [10].

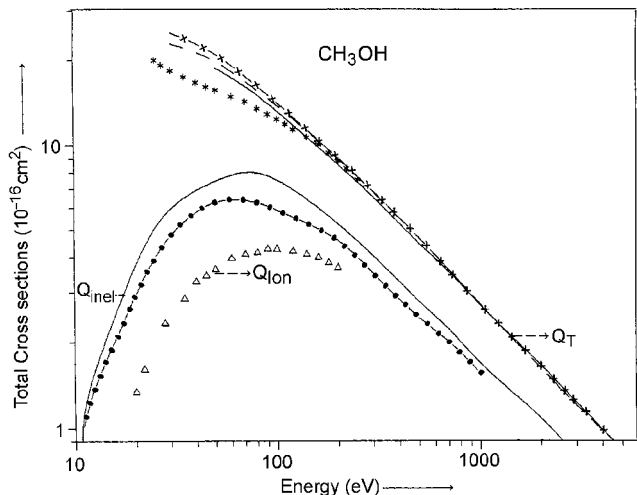


**Fig. 3.**  $e^-$ - $C_2H_6$  scattering: upper curves: ( $Q_T$ ) results in three present theories, same as in Figure 2; measurements ( $Q_T$ ): (□ □ □) reference [6], (Δ Δ Δ) reference [7], (☆☆☆) reference [4]; Lower curves: (—) present  $Q_{inel}$  (Eq. (8)), (-●-●-) theoretical  $Q_{Ion}$  reference [10], (○ ○ ○)  $Q_{Ion}$  measurements reference [9].

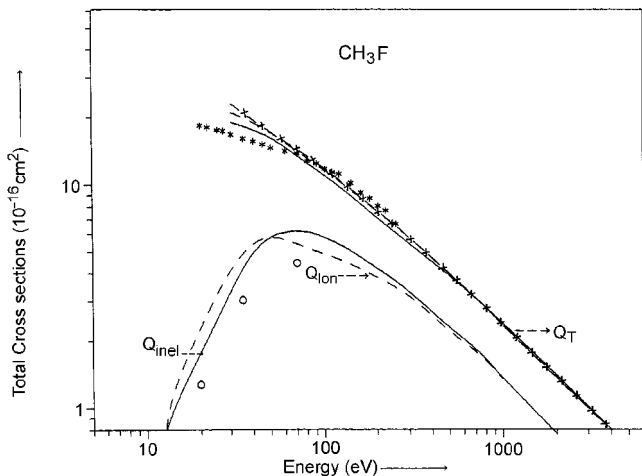
tramolecular scattering. These drawbacks are corrected for in the MAR and the MAR-SC formulations. The present work assumes interest also since we can obtain theoretical  $Q_{Ion}(M)$  as the high energy limit of  $Q_{inel}(M)$ .

#### $C_2H_2$ , $C_2H_4$ and $C_2H_6$ molecules

Total electron scattering cross-sections from these hydrocarbons have been examined against various other data in

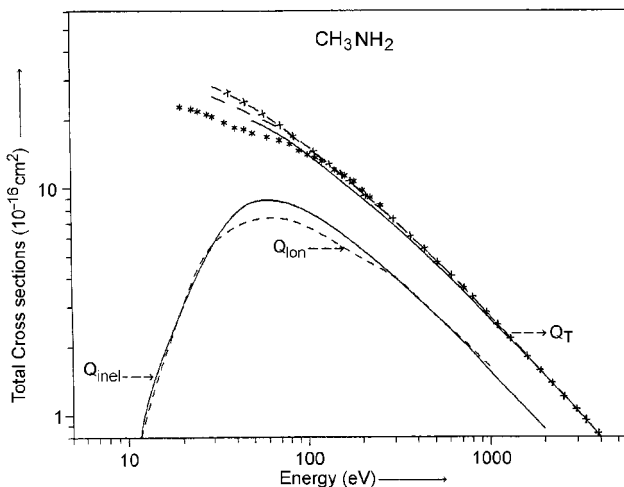


**Fig. 4.**  $e^-$ - $\text{CH}_3\text{OH}$  scattering: upper curves, present  $Q_T$  results same as in Figure 3, (\* \* \*) reference [7]; lower curves: (—) Present  $Q_{inel}$  (Eq. (8)), (-●-●-)  $Q_{Ion}$  (AR, Eq. (4)), ( $\Delta \Delta \Delta$ )  $Q_{Ion}$  measurements reference [22].



**Fig. 5.**  $e^-$ - $\text{CH}_3\text{F}$  scattering: Upper curves,  $Q_T$  same as in Figure 4, (\* \* \*) reference [7], lower curves: (—) present  $Q_{inel}$ , (- - -)  $Q_{Ion}$  in AR ( $\circ \circ \circ$ )  $Q_{Ion}$  measurements reference [23].

our Figures 1, 2 and 3. As shown in Figure 1 the complete TCS (upper curves) of acetylene molecules calculated by Jain and Baluja [11] using molecular orbitals, are higher than the present theoretical values and the experimental data of Sueoka and Mori [4] as well. Among the three present approaches the AR (Eq. (1)) overestimates the cross-sections upto about 1000 eV, as expected. The MAR is marginally better than the AR at energies below 100 eV. The two approximations tend to merge at high energies as the polarization contribution to the TCS becomes insignificant. Our MAR-SC calculations (Eq. (7)) based on the MAR for two effective scattering centers at carbon atoms in  $\text{C}_2\text{H}_2$ , yields  $Q_T$  values in good agreement with the measured data for  $E_i \geq 200$  eV. All the



**Fig. 6.**  $e^-$ - $\text{CH}_3\text{NH}_2$  scattering: theoretical curves, same as in Figure 5.

calculated values tend to coincide beyond 2000 eV, but on the whole our new method gives values in a better accord with the measured data.

We have also plotted here the molecular inelastic TCS  $Q_{inel}(M)$ , calculated in the present SC approach, *i.e.* equation (8). This compares well with the previous calculations [11]. The measured total ionization cross-sections  $Q_{Ion}$ , of Zheng and Srivastava [8] are lower than both the calculated values, at intermediate energies, since  $Q_{inel}$  includes  $Q_{Ion}$ . Towards high energies ( $\geq 200$  eV) these two quantities tend to merge as the ionization dominates the inelastic processes. Thus the calculated  $Q_{inel}$  serves as a high energy limit to  $Q_{Ion}$  in all the cases studied in this paper. Let us note that in the peak region (around 60 eV) the energy dependence of the measured  $Q_{Ion}$  (Fig. 1) differs from that of  $Q_{inel}$ . For the sake of clarity of the diagram we did not include here other ionization measurements, *e.g.* [21], but the measured values of Zheng and Srivastava [8] are somewhat higher than those of [21], at energies between 100 and 800 eV.

Consider now the  $e^-$ - $\text{C}_2\text{H}_4$  scattering vide Figure 2 wherein the only other theoretical result for  $Q_T$  is that of Jiang *et al.* [12]. These are higher than all the presently calculated values, upto 800 eV. This is due to the use of energy-independent polarization potential by Jiang *et al.* [12] as discussed by us in connection with  $e^-$ - $\text{H}_2\text{S}$  scattering [3]. The experimental TCS of Sueoka and Mori [4] are somewhat lower than those of Nishimura and Tawara at the lower end of energy (Fig. 2). The relative behaviour of AR and MAR is similar in all our Figures 1–6. There is a good agreement between the present MAR-SC results and the measured data [4,6] as shown in Figure 2. However the  $E_i$ -dependence of these measurements is somewhat different in the range 200–600 eV. All the compared data tend to a similar high energy limit. As far as the inelastic TCS of  $\text{C}_2\text{H}_4$  are concerned, the only comparable data are the theoretical  $Q_{Ion}$  of [10]. We believe that experimental data in this regard could fall in between these two (lower) curves.

In the case of  $C_2H_6$  (Fig. 3) other theoretical results on  $Q_T$  are similar to ours at large energies. Our own  $Q_T$  values in the three approaches mentioned earlier, exhibit a behavior like that of Figures 1 and 2. Of the three isocarbon molecules  $C_2H_2$ ,  $C_2H_4$  and  $C_2H_6$  the last one has the largest C–C bondlength (Tab. 1). This favours the approximations made and the three approaches AR, MAR and MAR–SC quickly tend to merge with increasing  $E_i$  as can be seen in Figure 3. Beyond 100 eV, our theories produce a better agreement with the experimental data of [7] and with [4] whereas the measurements of Nishimura and Tawara [6] are on the higher side. The data of [7] are found to lie between those of [5,6]. The cross-sections of  $C_2H_6$  are larger than those of the isocarbon  $C_2H_4$  molecule [5]. Further in Figure 3, the present  $Q_{inel}$  are seen to agree with the measured data on  $Q_{Ion}$ , given by Chatham *et al.* [9] as well as the model calculations of Hwang *et al.* [10], above 200 eV.

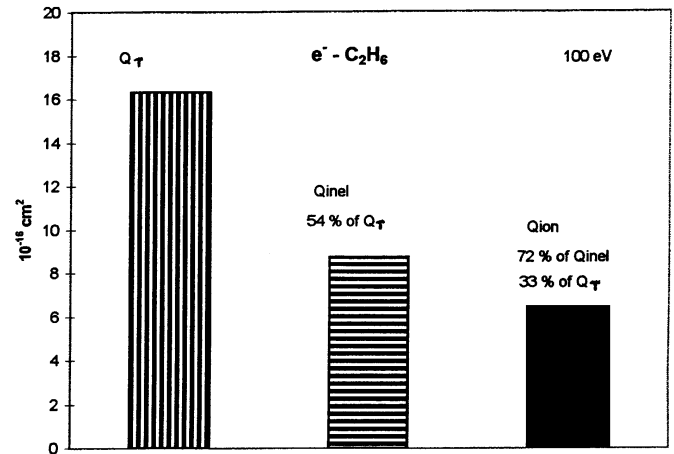
### CH<sub>3</sub>OH, CH<sub>3</sub>F and CH<sub>3</sub>NH<sub>2</sub> molecules

In these 18-electron targets the CH<sub>3</sub> group is typically bonded to X (= OH, F and NH<sub>2</sub>) through a relatively larger separation as mentioned earlier. The present work is aimed at providing theoretical total cross-sections at high energies, since the experiments [7] are limited to 250 eV only. Further there seem to be no calculations or measurements (except [22] for CH<sub>3</sub>OH) on electron impact ionization in these targets. In the case of CH<sub>3</sub>OH (Fig. 4) we find a good accord between our MAR–SC results and the experiments [7], beyond 100 eV. All our theoretical values mutually agree at large enough  $E_i$ . Figure 4 also exhibits the energy dependence of our  $Q_{inel}$  (Eq. (8)) vis-a-vis  $Q_{Ion}$  obtained in AR (Eq. (4)). The available ionization measurements [22] are lower than both the former values as expected. All the general comments about Figure 4 also apply to Figure 5 for CH<sub>3</sub>F and Figure 6 for CH<sub>3</sub>NH<sub>2</sub>. The ionization measurements [23] on CH<sub>3</sub>F (Fig. 5) being at three lower energies, are lower than  $Q_{inel}$  as well as  $Q_{Ion}$  (in AR). Our theoretical data can serve as a useful reference for the cross-sections on the present molecules at high impact energies. Among the 18-electron systems investigated here the  $C_2H_6$  molecule offers the largest cross-sections at a given energy. We have, therefore exhibited relative contributions of the elastic and inelastic cross-sections of  $C_2H_6$  in Figures 7a and 7b. At 100 eV the  $Q_{inel}$  and  $Q_{Ion}$  are 54% and 34% respectively of  $Q_T$ . At 1000 eV, these two cross-sections being practically the same, account for 58% of  $Q_T$ .

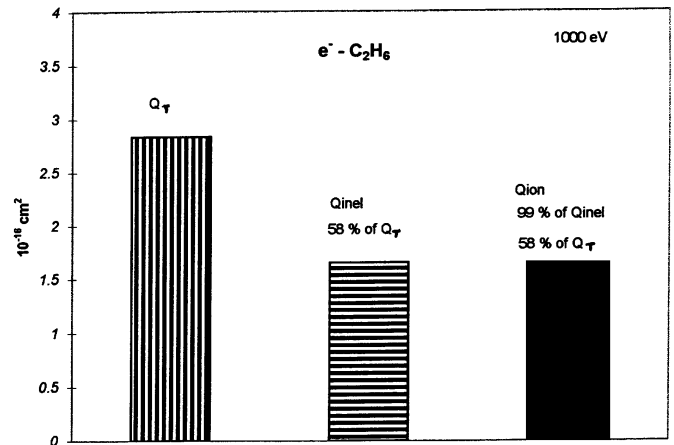
Now, let us briefly dwell upon the energy dependence of the  $e^-$ –*molecule* cross-sections  $Q_T$ . The behaviour predicted by Vogt and Wannier [24] on the basis of pure polarization potential was as follows

$$Q_T(E_i) = a\sqrt{\alpha_o/E_i}. \quad (9)$$

The cross-sections  $Q_{inel}$  or  $Q_{Ion}$  show a dependence as  $(\ln E_i/E_i)$  at high energies, but are also fitted to other



(a)



(b)

**Fig. 7.** (a) Relative contributions of various total cross-sections in  $e-C_2H_6$  scattering at 100 eV. (b) Same as in (a) but for 1000 eV.

forms. A short range Yukawa potential with Born approximation, yields a fitting relation [25],

$$Q_T(E_i) = a/(a + bE_i). \quad (10)$$

Our calculations in the present and the previous papers are based on the complex potential wherein the high energy behaviour is governed by the static and the absorption interactions. Hence we [2] fitted the TCS of 10-electron targets HF–H<sub>2</sub>O–NH<sub>3</sub>–CH<sub>4</sub> to the following general form

$$Q_T(E_i) = aE_i^{-b}. \quad (11)$$

We found that the parameter  $b$  was close to 0.7 for these targets. Let us now consider the 18-electron targets Ar and H<sub>2</sub>S together with CH<sub>3</sub>X investigated here and represent

**Table 2.** Parameters of the fitting formulas.

Target	Equation (11)		Equation (12)	
	$a$	$b$	$A$	$B$
Ar	117.9	0.56	108.4	0.56
H <sub>2</sub> S	171.3	0.61	82.3	0.61
CH <sub>3</sub> OH	257.3	0.64	126.1	0.64
CH <sub>3</sub> NH <sub>2</sub>	343.3	0.69	125.9	0.69
CH <sub>3</sub> F	335.3	0.70	149.1	0.70
C <sub>2</sub> H <sub>6</sub>	444.8	0.71	140.8	0.71

their TCS by an analytical fit,

$$\frac{Q_T}{a_o^2} = A \left( \frac{\alpha_o}{E_i} \right)^B \quad (12)$$

where  $a_o$  is the usual Bohr radius. In the energy range 100–1000 eV, the calculated cross-sections fit very well with the formula (12) and the corresponding parameters are exhibited in Table 2. The index  $B$  varies near 0.7 for these molecules. We further find that the dependence of  $Q_T$  on polarizability is also  $Q_T \sim \alpha_o^{0.7}$  as mentioned in [7]. However, as compared to 10-electron systems, the present 18-electron sequence from Ar atom onwards shows a slow variation in the index  $B$  (Tab. 2). The parameter  $A$  of equation (12) increases with typical bondlength of the molecule. The parameter  $A$  in equation (12) or  $a$  in (11) may itself be expressed in terms of the bond-length and the no. of electrons in the molecule but this is not attempted here. Rather, we have preferred to pull out the other molecular property  $\alpha_o$ , and express  $Q_T$  in terms of  $(\alpha_o/E_i)$ , in equation (12). The index  $B$  is  $\sim 0.7$  as compared to 0.5 in equation (9). Thus equation (9) predicted  $Q_T$  to be linearly varying with the time spent by the projectile in the target region, while our work shows a little faster variation.

## 4 Conclusions

This paper provides theoretical total cross-sections of electron scattering with C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub> and CH<sub>3</sub>X molecular targets, for comparison with various experimental and other data. The comparison has been satisfactory for all the targets at high impact energies. Apart from the AR and the MAR, we have developed here a variant of our previous work, called the MAR–SC which is useful for molecules (containing H-atom) where two scattering centers can be identified. This method is theoretically more satisfactory than that of Jiang *et al.* [13], who proposed empirical weighing of atomic contributions in the  $e$ -molecule cross-section. In any case, these modifications overestimate below 100 eV. The MAR–SC formulation based on groups of atoms in a molecule effectively utilizes molecular properties and can be extended to other targets like CH<sub>3</sub>CH<sub>2</sub>OH.

Further it appears that the  $Q_{inel}$  calculated presently and the  $Q_{Ion}$  obtained theoretically (*e.g.* Hwang *et al.* [10]) provide respectively the tentative upper and lower limits of the molecular ionization cross-sections in the range 100–1000 eV. The complete TCS are very well represented by formula (12) where one finds  $Q_T \sim (\alpha_o/E_i)^{0.7}$ . The present 18-electron systems show a systematic variation in the parameter  $A$  with respect to their bondlengths. The parameter  $B$  increases slowly in going from CH<sub>3</sub>OH to C<sub>2</sub>H<sub>6</sub> and is lower than that of the 10-electron systems.

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