

On trends in total cross sections for electron (positron) scattering on atoms and molecules at intermediate energies

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An examination of total electron and positron scattering cross sections in a large variety of atoms and molecules reveals a trend related to ground state target dipole polarizability. Some correlations of total cross section with diamagnetic susceptibility and the number of target electrons have also been noted. Experimental positron and electron cross sections between 100 and 500 eV can be reasonably well described by a simple formula based on polarizability and energy correlation.

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1. Introduction

Ever since the beginning of systematic investigations of scattering of electrons some efforts have been made [e.g. 1–4] to learn how the atomic and molecular structures are reflected in the magnitude and energetic dependence of cross section. So far, however, considerable attention has been paid to the manner in which the total cross sections of individual targets vary with the energy of projectile, and relatively little is to be found in the literature concerning the variation of total cross sections from target to target.

Lacking rigorous predictive calculations, one turns to searching for semiempirical correlations. Finding such correlations would allow to: first, predict the values of cross sections until experimental data are obtained, and second, could provide some stimulating insight into the role of microscopic target properties in the scattering process.

Most of the trends have been found so far in the region of thermal and low energies. Mean scattering cross section measured at very low energies [5] for *n*-alkanes vapours is comparable with the mean geometric cross section of the molecule and the cross sections for these molecules increase along with the increase of their polarizability. For polar molecules the magnitude of the momentum transfer cross section at low energies can be correlated to the permanent dipole moment of the molecule [6, 7]. Some correlations were also reported between the value of

cross section for ionization at a given energy (usually close to the cross section maximum) and such quantities as polarizability [8–10], diamagnetic susceptibility [10], mean square radii of atomic orbitals [11] or the number of *C* atoms in hydrocarbons [12].

Recently Floeder et al. [13] have measured the total cross sections for scattering of electrons and positrons on a large group of hydrocarbons and have observed an increase of cross section with the size of molecules. They have noticed that in the energy range between 100 and 400 eV total cross sections of hydrocarbons may be described as a linear function of the number of molecular electrons.

All these and other trends do not hold in general but only within a given target class or limited energy range.

A well known feature of total cross sections, common for atoms and molecules above 50 eV, both for electrons as well as positrons, is their decrease with the increase of scattering energy. Cross sections for electron are usually higher than those for positrons but at the highest energies investigated, there are indications [13, 47, 49, 59, 60] of a tendency towards merging of the positron and electron cross sections for respective atoms and molecules.

2. Procedure and results

The correlation of positron total cross sections at 100 eV with target polarizability is demonstrated in

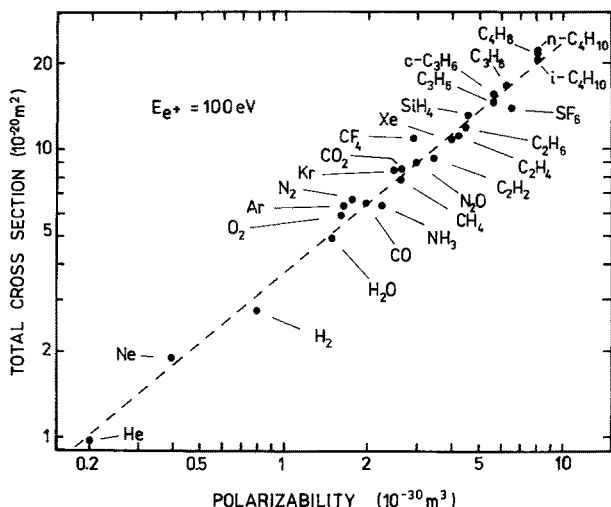


Fig. 1. Log-log plot of the experimental positron total scattering cross sections at 100 eV against the target static polarizabilities. Values of polarizabilities were taken from [70–74]. The experimental cross sections were obtained as weighted mean values of the cross sections taken from the following sources: He[46, 62, 65, 67], Ne[46, 63, 64, 66], Ar[46, 63, 66, 67], Kr[45, 48, 64], Xe[45, 48], H₂[47, 67–69], N₂[47, 67, 68], CO[49, 53, 67], O₂[52, 56, 68], H₂O[58], CO₂[47, 49, 53, 68], N₂O[50], CH₄[13, 52, 59, 68], NH₃[60], CF₄, SiH₄[55], C₂H₂[57], C₂H₄, C₂H₆[13, 59], SF₆[52], C₃H₆, *c*-C₃H₆, C₃H₈, C₄H₈, *i*-C₄H₁₀, *n*-C₄H₁₀ [13]. Least-squares line has been drawn through the points

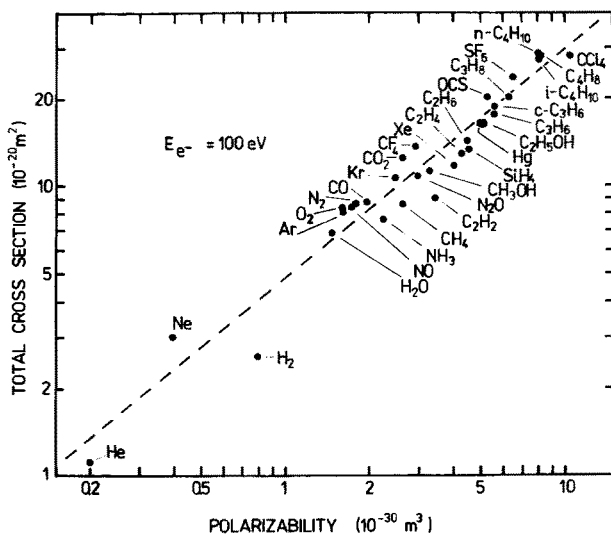


Fig. 2. Log-log plot of the experimental electron total scattering cross sections at 100 eV against the target polarizabilities. For references see Fig. 5. Least-squares line has been drawn through the points

Fig. 1. The distribution of points clearly suggests that total cross sections are usually greater for molecules of greater polarizability. The same type of graphs for other energies between 20 and 500 eV show a similar trend. However, in the case of electrons (Fig. 2) one

observes a slightly greater scatter of points in similar plots. It is interesting that the polarizability correlations for both projectiles have about the same slopes over a whole energy range studied.

On the ground of visible correlation between cross section and polarizability as well as energy dependence of cross sections, we have proposed the regression formula in the form:

$$Q(E) = 40 \cdot \alpha^{0.81} \cdot E^{-0.5} / (1 \pm 0.20 \cdot E^{-0.12}). \quad (1)$$

If polarizabilities α are in 10^{-30} m^3 and energies E in eV then the resulting cross sections $Q(E)$ are in 10^{-20} m^2 . The minus sign in (1) concerns electrons, while the plus sign applies to positrons.

The parameters in (1) have been evaluated with the use of a multiple least-squares fitting procedure. Fitting was done using the weighted mean values of all available experimental cross sections from the energy range of 100–500 eV for targets of polarizability below $11 \cdot 10^{-30} \text{ m}^3$. The weights of individual results were estimated on the basis of overall uncertainties of each experiment. The data for lower and higher energies were rejected in the process of fitting in order to treat the electron and positron cross sections on a similar basis. Below 100 eV, a significant contribution to the scattering is given by the exchange effect typical for electrons, and the positronium formation typical for positrons. On the other hand, above 500 eV there are far less experimental data for positrons than for electrons.

Deviations of the positron as well as electron total cross sections calculated using (1) from the experimental data for majority of targets (see Figs. 3 and 4) do not exceed the typical value of maximum experimental error. A greater deviation from the general trend for some compounds in case of electrons may partly result from the fact that results for electrons have been obtained using very different measurement techniques while for positrons, most of the measurements have been done using the time-of-flight set-up.

Between 20 and 100 eV, i.e. beyond the region of energies considered for fitting, cross sections calculated with the use of (1), are usually higher than the measured ones (Fig. 5) but still exhibit a trend similar to that observed at intermediate energies.

Concerning the energies higher than 500 eV we must stress that the semiempirical electron and positron cross sections for a given target merge with energy much more slowly than do experimental data. However, an examination of available experimental data suggests that, in general, the $E^{-0.5}$ dependence holds also at high energies.

It is worth mentioning that the proposed energetic dependence of the cross section is very close to the

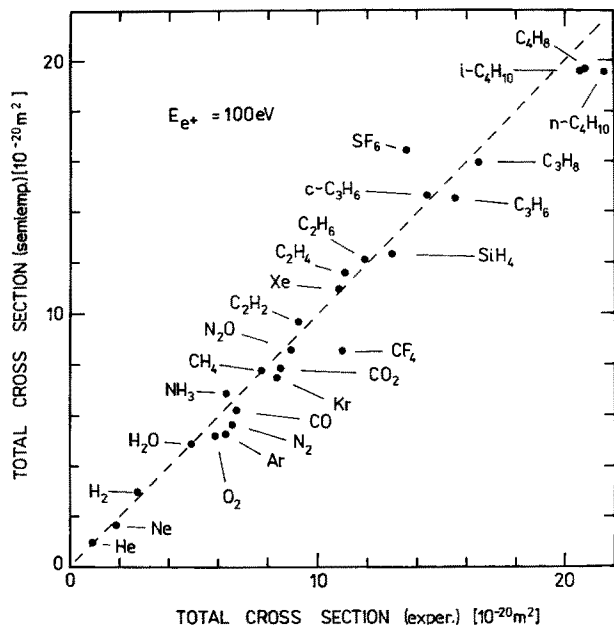


Fig. 3. Plot of the calculated (according to (1)) positron cross sections at 100 eV versus the experimental total cross sections. The broken line represents the case of perfect agreement between calculated (semiempirical) and experimental cross sections. For references see Fig. 1

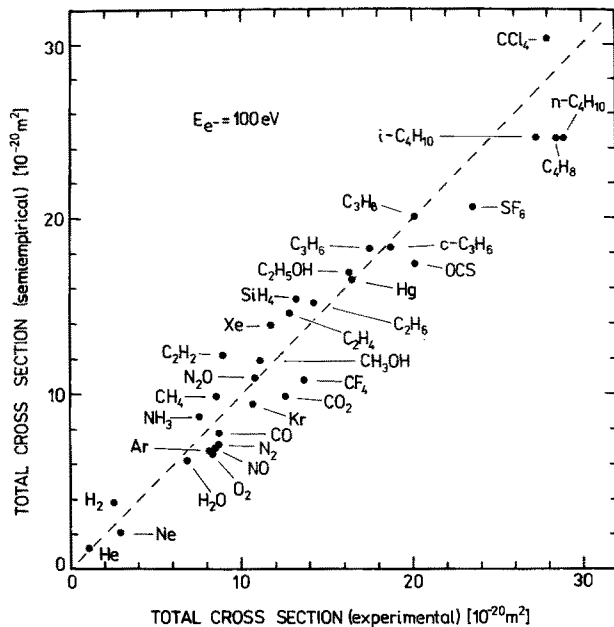


Fig. 4. Plot of the calculated (with the use of (1)) electron cross sections at 100 eV versus the experimental total cross sections. The broken line represents the case of perfect agreement between semiempirical cross sections and experimental data. For references see Fig. 5

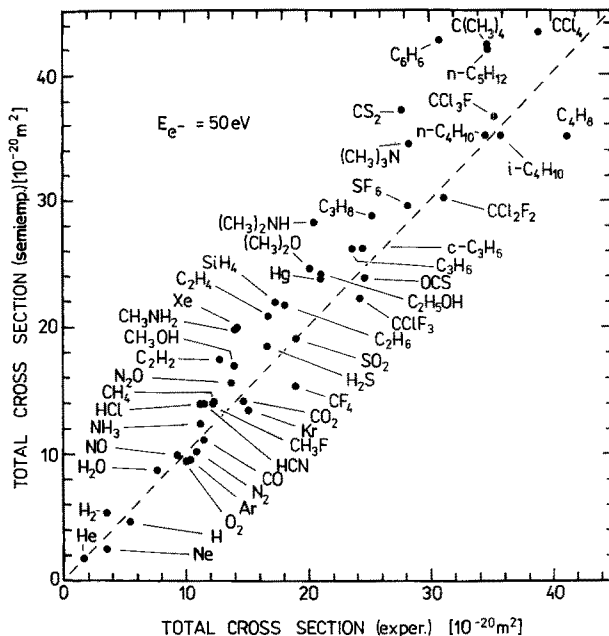


Fig. 5. Plot of the calculated (with the use of (1)) electron total cross sections at 50 eV versus the experimental cross sections. The experimental cross sections are the weighted mean values of the data taken from the following sources: H[16], He[18, 22, 26, 32, 46], Ne[24, 31, 32, 36, 46], Ar[24, 25, 32, 36, 46], Kr[24, 25, 36, 45, 48], Xe[24, 25, 32, 36, 45, 48], Hg[21], H2[23, 27, 33, 47, 69], N2[20, 22, 28, 36, 43, 47, 53], CO[1, 49, 53], NO[1, 28], O2[1, 17, 28, 29, 52, 56], HCl(extrapol.) [1], H2O[2, 14, 30, 39, 58], CO2[1, 40, 47, 49, 53], N2O[1, 42, 50], H2S[38], SO2[37, 51], OCS[42, 51], CS2[41], NH3[2, 42, 60], C2H2[3, 14, 57], CH4[4, 13, 34, 36, 52, 55, 59], CF4[35, 55], SiH4[55], CClF3, CCl2F2, CCl3F[35], CCl4[35, 61], C2H4[3, 13, 59], CH3OH, C2H5OH[14, 54], SF6[19, 52], C2H6[4, 13, 59], C3H6, *c*-C3H6, C4H8[13], C3H8[4, 13], *i*-C4H10, *n*-C4H10[4, 13, 14], *n*-C5H12[14], C6H6(extrapol.) [15], HCN, CH3F, CH3NH2, (CH3)2NH, (CH3)2O, (CH3)3N, C(CH3)4 [14]. The broken line represents the case of perfect agreement between semiempirical and experimental cross sections

classical result for pure asymptotic polarization potential (see in [75]) as well as to that in semiempirical formula of Floeder et al. [13]. Such energy dependence suggests that at intermediate energies the total cross section is, within a good approximation, proportional to the time the projectile spends in vicinity of the target.

Available data for highly polarizable targets, eg. sodium atoms [76], sodium dimers [77], potassium atoms [76, 78] and potassium dimers [77], with polarizabilities [74] of 24, 30, 43 and $60 \cdot 10^{-30} \text{ m}^3$, respectively, indicate that polarizability correlation may hold also for species with polarizabilities much higher than taken into fitting.

One would expect some correlation between total cross section and polarizability because certain polarizability correlations have been earlier found [8–10] for electron ionization cross section at energies close

to the maximum and in the considered energy range electron ionization cross sections constitute nearly half of the corresponding total cross sections. However, while total cross sections of examined targets show a single correlation with polarizability in a very wide energy range, the near-maximum ionization cross sections of different classes of targets form separate linear correlations [10].

Further examination of experimental data show that, approximately, total cross section tends also to be greater for targets of greater absolute value of diamagnetic susceptibility (values of χ_m taken from [79]) and, to a much lesser degree, for targets with higher number of electrons. It seems, however, that the available data do not fall in single correlations with any of these two target properties but rather form separate linear correlations within selected groups of target (e.g. noble gas atoms, hydrocarbons [13] and chloro-fluoromethanes).

3. Conclusion

By examining the available experimental total electron and positron scattering cross sections for a number of various targets we have found that at intermediate energies the total cross section shows significant correlation with ground state target dipole polarizability. In contrast to the single polarizability correlation, several separate correlations with diamagnetic susceptibility and the number of target electrons for selected classes of targets have been observed. Because the valence electrons make the greatest contribution to the polarizability (diamagnetic susceptibility) of targets it seems that the noticed trends reflect an importance of the external, most loosely bound, target electrons in scattering process.

We have designed a simple formula which reproduces most of the experimental data with an accuracy comparable to their uncertainties. This formula may be useful for rough estimation of total cross sections for species lacking experimental data (especially due to experimental difficulties), provided that the polarizability of the target is measured or calculated.

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