

A new semi-empirical formula for total cross sections of electron scattering from triatomic molecules at 30—5000 eV

Deheng Shi (施德恒)^{1,2}, Yufang Liu (刘玉芳)², Jinfeng Sun (孙金锋)², and Zunlue Zhu (朱遵略)²

¹College of Physics and Electronic Engineering, Xinyang Normal University, Xinyang 464000

²Department of Physics, Henan Normal University, Xinxiang 453007

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Total cross sections (TCSs) of electrons scattering from triatomic molecules over the energy range from 30 to 5000 eV are investigated employing a new semi-empirical formula. The TCSs of electrons scattering from triatomic molecules SO₂, NO₂, and CO₂ are calculated. The quantitative TCSs are in good agreement with those obtained by experiments. It is shown that the results derived from the semi-empirical formula are much closer to the measurements than other calculations.

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Total cross sections (TCSs) for electrons scattering from molecules over a wide energy range are widely used in gaseous lasers, astrophysics, plasma physics, atmospheric physics, and chemical physics, etc.. TCS values reproduced by analytical or empirical expressions accurately are very useful in computational work related with these applications. Because electron-molecule scattering is a much more complex problem than the corresponding electron-atom scattering, in order to get more accurate TCSs, many approaches were presented^[1–3] in the past decades. Here, over the intermediate- and high-energy ranges, since almost all inelastic channels (rotational, vibrational, electronic excitation, and ionization process, etc.) are open, a conventional close-coupling theory for electron-molecule scattering is almost impossible to be established. Because of the lack of accurate calculation methods, great discrepancies of TCSs exist between theories and measurements at intermediate and high energies.

For the above-mentioned reasons, recently, many approximate methods, such as the additivity rule (AR) model^[4], the modified AR model^[5,6], the independent atom model (IAM)^[7], the two-parameter formula^[8], the spherical complex optical potential (SCOP)^[9], and the modified potential method^[10–12], were proposed. In this letter, we investigate the semi-empirical formula for simple diatomic molecules, develop it into equations suitable for some triatomic molecules, and calculate the TCSs of electrons scattering from several triatomic molecules such as SO₂, NO₂, and CO₂.

By investigating the TCSs derived from the AR model^[4–6], we find the relations between TCS and the incident energy of electrons, which are identical with the first Born approximation. That is to say, if $E \rightarrow \infty$, then

$$\sigma_T(E) \rightarrow AE^{-1}. \quad (1)$$

Considering the energy dependence in the Born approximation formula, and analyzing a large number of experimental data and theoretical results, the TCSs of electrons scattering from simple diatomic molecules over the intermediate- and high-energy ranges are attained as

$$\sigma_T(E) = \frac{d\sigma_0}{d + C\sigma_0 E}, \quad (2)$$

where E is the energy of the incident electron in eV; C is a fitting parameter; $\sigma_T(E)$ is the TCS at energy E , d ($\times 0.1$ nm) and σ_0 ($\times 0.01$ nm²) are two free parameters for a particular molecule, which can be fitted by two points of energy and the corresponding TCSs, σ_0 is the TCS corresponding to zero impact energy.

Let $C = 5.5 \times 10^{-3}$ (eV·nm)⁻¹. By using Eq. (2), we have fitted the TCSs of electrons scattering from CO, NO, O₂, HCl, and N₂ and found $d \approx 2r_0$. This means that the TCSs of electrons scattering from diatomic molecules depend on the internuclear distance r_0 between two atoms. In the formula, we label the electron-molecule interactions as a “hard sphere” potential with radius r_0 . So, the TCS of zero energy would be equal to $4\pi r_0^2$ ^[13]. We obtain a semi-empirical formula

$$\sigma_T(E) = \frac{4\pi r_0^2}{1 + C \cdot 2\pi r_0 E}. \quad (3)$$

Obviously, the TCSs depend on a unique parameter r_0 . The TCSs of electrons scattering from simple diatomic molecules can be calculated by Eq. (3).

Now, we develop Eq. (3) into the form suitable for the TCS calculations of electrons scattering from triatomic molecules which have C_{2v} or $D_{\infty h}$ symmetry. For simplicity, we only take into account three molecules (SO₂, NO₂, and CO₂) in this letter. For these molecules, the maximum scale along the bond axis between the central atom and the any other one (i.e., S—O bond for SO₂, N—O for NO₂, and C—O for CO₂) equals the bond length r_0 . Therefore, when we neglect the long-distance interactions of electrons with triatomic molecules such as SO₂, NO₂, and CO₂, we can also set $d = 2r_0$ and treat their interactions roughly as a “hard sphere” potential with radius r_0 for Eq. (2). So Eq. (3) for TCSs of electrons scattering from SO₂, NO₂, and CO₂ over the intermediate- and high-energy range is appropriate.

Using Eq. (3) and $r_0 = 0.14308$ nm for SO₂, $r_0 = 0.1193$ nm for NO₂, and $r_0 = 0.1160$ nm for CO₂^[14], we have calculated the TCSs of electrons scattering from these molecules at 30—5000 eV. The calculations together with the measurements, recent theories obtained

by the modified potential method, and the results of the empirical formula given by García *et al.*^[8] are shown in Figs. 1—3, respectively. The present semi-empirical calculation results are shown in Table 1. Atomic units are employed throughout in this letter if not specified.

Figure 1 shows the TCSs for e-SO₂ scattering together with the measurements obtained by Zecca *et al.*^[15] over 90—4000 eV and Szmytkowski *et al.*^[16] over 30—70 eV, the results of the empirical formula given by García *et al.*^[8] at 30—5000 eV, the theories obtained by Raj *et al.*^[7] over 100—4000 eV, and the calculations derived from the modified and unmodified potential methods^[10–12] over 30—5000 eV. From Fig. 1, we can easily see that the present results agree well with all the measurements^[15,16] at the corresponding energy ranges, the data derived from the modified potential method^[10–12], and the calculation results derived from the empirical formula given by García *et al.*^[8] at higher energies. Obviously, Eq. (3) is completely suitable for the TCS calculations of e-SO₂ scattering at 30—5000 eV.

Figure 2 shows the present e-NO₂ TCSs together with the calculations obtained by Joshipura *et al.*^[17] at 100—1000 eV, the theories given by the empirical formula of García *et al.*^[8] and our modified and unmodified potential methods^[10–12] at 30—5000 eV, and the measurements obtained by Zecca *et al.*^[15] at

100—4000 eV and Szmytkowski *et al.*^[18] at 30—220 eV. Obviously, the present results agree very well with all the measurements at the corresponding energy ranges. For example, the largest discrepancies between Zecca's measurements^[15] and the present results, and between

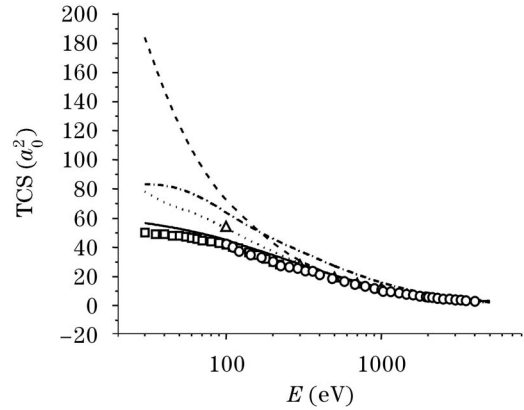


Fig. 2. TCSs for e-NO₂ scattering. Theories: solid line, present semi-empirical results; dashed line, García empirical results^[8]; dotted line, results derived from modified potential; dash-dotted line, results from unmodified potential; triangles, Joshipura *et al.*^[17]. Experiments: circles, Zecca *et al.*^[15]; squares, Szmytkowski *et al.*^[18].

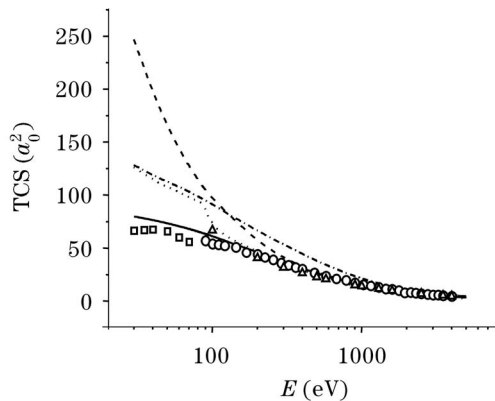


Fig. 1. TCSs for e-SO₂ scattering. Theories: solid line, present semi-empirical results; dashed line, García empirical results^[8]; dotted line, results derived from modified potential; dash-dotted line, results from unmodified potential; triangles, Raj *et al.*^[7]. Experiments: circles, Zecca *et al.*^[15]; squares, Szmytkowski *et al.*^[16].

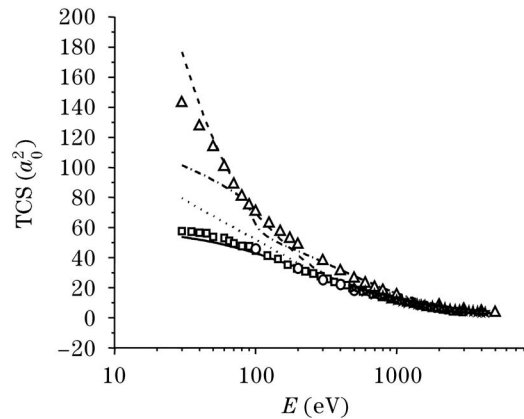


Fig. 3. TCSs for e-CO₂ scattering. Theories: solid line, present semi-empirical results; dashed line, García empirical results^[8]; dotted line, results derived from modified potential; dash-dotted line, results from unmodified potential; triangles, Jain *et al.*^[9]. Experiments: squares, Szmytkowski *et al.*^[19]; circles, Kwan *et al.*^[20]; stars, Xing *et al.*^[21].

Table 1. TCSs for Electron Scattering from SO₂, NO₂, and CO₂ in Units of a₀²

Energy (eV)	SO ₂	NO ₂	CO ₂	Energy (eV)	SO ₂	NO ₂	CO ₂	Energy (eV)	SO ₂	NO ₂	CO ₂
30.0	80.05	56.88	53.94	400.0	30.87	24.13	23.21	1800.0	9.29	7.59	7.35
40.0	76.75	54.86	52.07	500.0	26.48	20.88	20.11	2000.0	8.44	6.91	6.70
50.0	73.71	52.99	50.34	600.0	23.18	18.40	17.74	2250.0	7.58	6.22	6.03
60.0	70.90	51.24	48.71	700.0	20.61	16.45	15.88	2500.0	6.88	5.65	5.48
70.0	68.29	49.60	47.18	800.0	18.55	14.87	14.36	2750.0	6.30	5.18	5.03
80.0	65.87	48.06	45.75	900.0	16.87	13.57	13.11	3000.0	5.81	4.78	4.64
90.0	63.62	46.62	44.40	1000.0	15.46	12.48	12.06	3500.0	5.02	4.14	4.02
100.0	61.51	45.25	43.13	1200.0	13.26	10.75	10.40	4000.0	4.42	3.65	3.55
200.0	46.22	35.03	33.54	1400.0	11.60	9.44	9.14	4500.0	3.95	3.27	3.17
300.0	37.02	28.57	27.43	1600.0	10.32	8.41	8.15	5000.0	3.57	2.96	2.87

Szmytkowski's measurements^[18] and the present results are 15.1% and 16.1%, respectively. Above 4000 eV, to our knowledge, there are no experimental data to be compared. But according to the excellent agreement over 30—4000 eV, we conclude that the e-NO₂ scattering TCSs must be accurate over 4000—5000 eV.

As shown in Fig. 3, the present TCSs are in excellent agreement with the measurements obtained by Szmytkowski *et al.*^[19] over 30—2916 eV, Kwan *et al.*^[20] over 100—500 eV, Xing *et al.*^[21] over 500—4250 eV, and the theories obtained by Jain *et al.*^[9], the empirical results of García *et al.*^[8] and our modified potential method^[10–12] at higher energies. But we also easily see that there are large discrepancies between the theories obtained by Jain *et al.*^[9], the results of the empirical formula given by García *et al.*^[8], the unmodified potential method^[10–12], and the measurements^[19–21] at lower energies, especially below 500 eV.

Obviously, as shown in Figs. 1—3, our semi-empirical method can give more accurate TCS results than that of García *et al.*^[8], and exceeds all the other theoretical methods in accuracy over a wide energy range, especially at lower energies. Thus, we can say that our present semi-empirical method is very encouraging.

From the above discussion of e-SO₂, -NO₂, and -CO₂ scattering, we easily see that Eq. (3) can give very accurate TCS results. Because this approximation only takes into account the short-range interactions of electrons with molecules and neglects the long-range interactions, the discrepancies between the values derived from Eq. (3) and the measurements remain in Figs. 1—3. At the same time, the long-range interactions are different from each other, the discrepancies remain and differ from each other.

Equation (3) is suitable for the TCS calculations of triatomic molecules which have C_{2v} or $D_{\infty h}$ symmetry. As further investigation in progress, we will develop it into equations suitable for TCS calculations of complex molecules, such as spherical polyatomic molecules.

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