## Additivity rule for the calculation of electron scattering from polyatomic molecules

Yuhai Jiang,<sup>1,2</sup> Jinfeng Sun,<sup>1,2</sup> and Lingde Wan<sup>2</sup>

<sup>1</sup>CCAST (World Laboratory), P.O. Box 8730, Beijing 100080, China

<sup>2</sup>College of Physics and Information Engineering, Henan Normal University, Xinxiang 453002, China\*

(Received 2 May 2000; published 10 November 2000)

Total cross sections (TCSs) for electron scattering by polyatomic molecules  $C_2F_4$ ,  $C_2F_6$ ,  $C_3F_6$ ,  $C_3F_8$ ,  $C_6F_6$ , and  $C_6H_6$  are calculated in the incident electron energy range 30–3000 eV employing the 100% additivity rule and energy-dependent geometric additivity rule (EGAR) approaches. The EGAR, proposed by Jiang *et al.* [J. Phys. B **30**, 5025 (1997); Phys. Lett. A **237**, 53 (1997)], relates to molecular properties and the energy of incident electrons. Two approaches for the TCS of  $C_2F_6$ ,  $C_3F_8$ ,  $C_6F_6$ , and  $C_6H_6$  molecules are compared and the EGAR yields better accord with available experimental measurements in the whole energy region. The new results for  $C_2F_4$  and  $C_3F_6$  are also presented although no experimental data are available for comparison. The atoms are presented by spherical complex optical potential, which is composed of static, exchange, polarization, and absorption terms.

PACS number(s): 34.80.Bm

#### I. INTRODUCTION

In recent years, more and more experimental and theoretical researches focus on the total cross sections (TCSs) for electron scattering by molecules in the intermediate- and high-energy region. On one hand, fundamental molecular properties of electron collision processes can be used to assess the behavior of molecules in its use for applications, such as for a variety of plasma-assisted material-processing applications and manufacturing semiconductor devices [1]. On another side, there is a special interest for the search for systematic relations between the TCS and other molecular parameters. For these reasons, in the last few years the number of works devoted to the TCS measurements for impact energies up to 5000 eV has been increasing [2-5]. In case of e-molecule scattering, this is a more complex problem than *e*-atom scattering due to the multicenter nature, the lack of a center of symmetry and nuclear motion. In addition, at intermediate and high energies, almost all inelastic channels (excitation, ionization, rotation, vibration, etc.) are open, which makes an ab initio calculation almost impossible. In the present energy region concerned, the additivity model [6-15] is a successful approach, which ignores anisotropic e-molecule interactions, and the molecular problem is reduced to the atomic problem, which is easier to handle. In the last 20 years, the additivity rule (AR) has been employed widely in the molecular calculation of electron impact ionization cross sections [6], photoionization cross sections [7], polarizabilities [8], positron scattering cross sections [9], as well as the ionization cross sections of electron-cluster collision [10] shown in Table I. For the determination of the total cross section for electron scattering from molecules, many calculations have been completed by employing the additivity model and the results are more interesting [11– 15], particularly for simpler and smaller molecules in the intermediate- and high-energy region (about E > 100 eV). However, the additivity rule (AR) results on some complex molecules (such as  $C_nH_m$  molecules), show larger discrepancies than those on diatomic and triatomic molecules at the same incident energies [14]. Here, we consider the AR employed in Refs. [11–15] as the 100% AR.

In the most recent papers some progress has been made in extending 100% AR validity to lower energies. Joshipura and Patel [16] separated the polarization interaction from the optical potential, and then obtained atomic cross sections from the remaining short-range interactions. Then, they summed atomic cross sections with the cross section for scattering on the molecular polarization potential. Employing this approach, they calculated the TCS for simple diatomic molecules and improved their results in a way. In 1997, in order to extend 100% AR to the application on larger molecules, we [17,18] improve the 100% AR model considering molecular geometric properties and propose an energydependent geometry additivity rule (EGAR). This approach had been employed in the calculation of TCS for electron scattering from CO<sub>2</sub>, CS<sub>2</sub>, N<sub>2</sub>O, NH<sub>3</sub>, SF<sub>6</sub> [17], and C<sub>n</sub>H<sub>m</sub> [18] molecules and the results are satisfactory. In this paper, we employ the 100% AR and EGAR to calculate the TCS of electron scattering from C<sub>2</sub>F<sub>4</sub>, C<sub>2</sub>F<sub>6</sub>, C<sub>3</sub>F<sub>6</sub>, C<sub>3</sub>F<sub>8</sub>, C<sub>6</sub>F<sub>6</sub>, and  $C_6H_6$  molecules in the incident energy 30-3000 eV region in order to verify further the present approaches and support the experimental data. In experiments, the group of Szmytkowski and co-workers [19-21] has quite recently completed their measurements using electron-transmission experiments for impact energies 1-250 eV for C<sub>2</sub>F<sub>6</sub> [19], 0.6-250 eV for C<sub>6</sub>F<sub>6</sub> [20] and 0.6-3500 eV for C<sub>6</sub>H<sub>6</sub> [21]. In addition, Sueoka [22] has determined the TCS for electron scattering from  $C_6H_6$  at energies from 1 to 400 eV using a strong, longitudinal guiding magnetic field. For the C<sub>3</sub>F<sub>8</sub> molecule, Kimura and co-workers [23] have reported recently the measured data on the TCS between 0.7 and 600 eV. No experimental measurements are available for the TCS on C<sub>2</sub>F<sub>4</sub> and C<sub>3</sub>F<sub>6</sub> molecules in the present energy region in the literature. Also, we are not aware of other theoretical researches for the TCS on these polyatomic molecules in the present energy region.

<sup>\*</sup>Address for correspondence. Email address: yhjiang@371.net

TABLE I. Total cross sections (TCSs) of molecules, which are obtained by the present AR and EGAR approaches in units of  $10^{-20} m^2$ .

Energy (eV)	TCS(C <sub>2</sub> F <sub>4</sub> ) AR EGAR	$TCS(C_2F_6)$ AR EGAR	$TCS(C_3F_6)$ AR EGAR	TCS(C <sub>3</sub> F <sub>8</sub> ) AR EGAR	$TCS(C_6F_6)$ AR EGAR	$\frac{\text{TCS}(\text{C}_6\text{H}_6)}{\text{AR EGAR}}$
30	42.20 33.57	52.67 36.36	63.29 43.44	73.77 48.82	95.18 71.38	81.74 65.84
40	39.15 31.93	49.21 35.04	58.72 41.94	68.79 46.97	87.23 67.10	72.74 60.32
50	36.36 30.25	45.98 33.62	54.54 40.23	64.15 45.03	80.23 63.04	65.26 55.33
60	33.78 28.56	42.96 32.12	50.67 38.39	59.85 43.00	73.81 59.05	58.64 50.59
70	31.58 27.06	40.35 30.76	47.37 36.69	56.14 41.17	68.44 55.61	52.78 46.60
80	29.82 25.86	38.21 29.66	44.73 35.31	53.11 39.71	64.30 52.95	49.20 43.55
90	28.31 24.80	36.36 28.67	42.47 34.08	50.51 38.42	60.80 50.66	45.85 40.99
100	27.02 23.89	34.75 27.80	40.53 32.99	48.26 37.28	57.88 48.74	43.14 38.89
200	18.83 17.51	24.39 21.23	28.25 24.92	33.80 28.70	39.84 35.72	27.78 26.17
300	14.56 13.83	18.91 17.10	21.85 19.97	26.19 23.23	30.67 28.31	20.77 19.92
400	12.09 11.62	15.76 14.56	18.14 16.91	21.80 19.83	25.30 23.75	16.65 16.13
500	10.33 10.00	13.51 12.65	15.50 14.63	18.67 17.26	21.44 20.35	13.78 13.44
600	9.00 8.75	11.80 11.16	13.50 12.86	16.30 15.24	18.63 17.82	11.75 11.49
700	8.01 7.82	10.52 10.02	12.01 11.52	14.53 13.70	16.49 15.86	10.21 10.02
800	7.16 7.00	9.43 9.03	10.73 10.34	13.01 12.34	14.65 14.15	8.94 8.79
900	6.51 6.38	8.59 8.26	9.76 9.44	11.84 11.30	13.27 12.87	8.09 7.97
1000	6.02 5.91	7.95 7.68	9.03 8.76	10.96 10.50	12.25 11.91	7.48 7.38
2000	3.49 3.46	4.66 4.57	5.24 5.16	6.40 6.26	6.97 6.87	3.90 3.87
3000	2.29 2.27	3.09 3.05	3.43 3.39	4.23 4.17	4.45 4.41	2.29 2.28

# II. ADDITIVITY RULE AND COMPLEX OPTICAL POTENTIAL

In the 100% additivity rule (AR) [11-15], the implicit assumption is made that molecular orbitals can be described by the sum of the valence orbitals of all atoms presented in the molecule. As a result, the TCS of *e*-molecule scattering is written as the sum of the TCS of atoms. Thus, the molecular cross sections according to the 100% AR are given by

$$Q_{MA}(E) = \frac{4\pi}{k} \operatorname{Im} F_m(\theta = 0) = \frac{4\pi}{k} \operatorname{Im} \sum_{j=1}^{N} f_j(\theta = 0)$$
$$= \sum_{j=1}^{N} q_T^j(E), \qquad (1)$$

where  $q_T^j$  and  $f_j$  are the TCS due to the *j*th atom of the molecule and the complex scattering amplitude for constituent atoms of the molecule, respectively. We can see that in the 100% AR, Eq. (1), one main effect is not considered: a close-packed molecule is not fully transparent for lowenergy electrons (about E < 100 eV) and the "inner" atoms are shielded by the "outer" atoms and do not contribute to the molecular cross sections. The shielding effect, which leads to smaller molecular scattering cross section than that predicated by the 100% AR, is dependent on the geometry of the molecule and introduces an orientational dependence in the scattering cross section of nonspherically symmetric molecules. The incorporation of molecular orbitals and shielding in molecules is difficult to achieve theoretically. Bobeldijk et al. [7] incorporated the shielding effect in the additivity of the ionization cross section of atomic units or subunits of the

molecules and presented a geometric additivity rule (GAR). We notice that the GAR model, which incorporates geometry of the molecule, is a good approach and can also be applied to the calculation of the TCS for *e*-molecule scattering, particularly for complex polyatomic molecules at low and intermediate energies [18]. However, we know that a closepacked molecule is not fully transparent for low-energy electrons, but the transparency will improve as incident electron energy increases. When the incident electron energy is appropriately high, the molecule should be fully transparent and each atom in the molecule can be freely scattered, there the 100% AR (1) is valid. This property cannot be in the GAR model. Thus the GAR gives a poor shape of cross sections compared with experiments in a wide incident electron energy range for polyatomic molecules, which has been seen by the calculation of the TCS for  $CO_2$ ,  $NO_2$ ,  $CS_2$ , SF<sub>6</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>3</sub>H<sub>6</sub>, etc. molecules in Refs. [17,18]. So, we [17,18] assume that "inner" atoms are shielded perfectly by "outer" atoms at  $E \rightarrow 0$  eV, at which the GAR presents reasonable results and at high-energy energies the 100% AR is a correct approach for the TCS. Considering the above factors, we incorporate the 100% AR and GAR, and present semiempirically an energy-dependent geometric additivity rule (EGAR). According to Jiang et al. [17,18], here we assume a cylindrical symmetry for the  $C_n F_m$  and  $C_6 H_6$ molecules under study. Linear molecules are approximated by a rodlike shape; circular molecules are approximated by a toruslike shape. The molecular cross sections  $Q_{MT}(E)$  according to the EGAR are written as

$$Q_{MT}(E) = Q_{MG}(E) + A(Q_{MA}(E) - Q_{MG}(E)), \qquad (2)$$

where  $Q_{MG}(E)$  is a molecular cross section in the GAR, which is given [7]

$$Q_{MG}(E) = \frac{1}{3}Q_{\parallel}(E) + \frac{2}{3}Q_{\perp}(E).$$
(3)

 $Q_{\parallel}(E)$  and  $Q_{\perp}(E)$  are the TCS for the electron approaching the molecule parallel to the z axis ( $\theta = 0$ ) and the TCS for an approach perpendicular to the z axis ( $\theta = \pi/2$ ), separately (reading Refs. [7] for details). In this paper, in the case of linear molecules, the subunits are the CF, CF<sub>2</sub>, and CF<sub>3</sub> groups. This means that  $Q_{\parallel}(E)$  and  $Q_{\perp}(E)$  are set equal to the cross section of a unit and the sum of the cross sections of "outer" sub-units, respectively. For example, the  $C_2F_4$ molecule is approximated by a rodlike shape and z-axis is attached to the axis of the symmetry. So,  $Q_{\parallel}(E)$  and  $Q_{\perp}(E)$ in Eq. (3) equal to  $Q_{CF_2}$  and  $Q_{CF}+Q_{CF}$ , respectively. The cross sections of  $Q_{CF_2}$  and  $Q_{CF}$  can be obtained by the 100% AR [Eq. (1)]. The A in Eq. (2) is and energy-dependent correction factor to merge with the 100% AR at high energies. We assume that

$$A = \frac{E}{mC + E},\tag{4}$$

where E in unit of eV is incident electron energy. The m is the number of electrons in the molecule. We let C=1 in units of eV considering the reasonable dimension relation. Here, the A is an empirical fraction that exhibits the TCS contribution of shielded atoms for different molecules at different energies. The formal calculations of the contribution of shielded units or subunits to the TCS are highly complicated by the geometry and composition of the molecule as the incident energies are varied [7]. Choosing the A, three factors are considered. First, the A should satisfy

$$Q_{MT}(E) \approx \begin{cases} Q_{MG}(E) & \text{if } E \to 0 \ A \to 0 & \text{(the GAR),} \\ Q_{MA}(E) & \text{if } E \to \infty \ A \to 1 & \text{(the 100% AR).} \end{cases}$$
(5)

Secondly, according to Eq. (4), at the same incident energy the more complex the molecule is, the smaller the A is. We can find that the C<sub>6</sub>F<sub>6</sub> molecule shows more shielded cross sections than the C<sub>6</sub>H<sub>6</sub> molecule at same incident energies. For example, the shielded cross sections account for 19% for  $C_6H_6$  and 25% for  $C_6F_6$  at 30 eV. It is reasonable because the F atom provides a larger contribution for shielding effect than the H atom in the same geometric molecule. Third, the empirical fraction A is related to E and m without any adjusted parameters and ensures the reasonable shape for the TCS against experimental data in the wide energy range. The form of the A has also been discussed in detail and these characters have also been shown by the calculation on the TCS for many molecules in previous work [17,18]. In this paper, the cross section of each unit can be obtained by 100% AR [Eq. (1)]. The  $q_T^j(E)$  of Eq. (1) for the *j*th atom is obtained by the method of partial waves:

$$q_T^j(E) = q_e^j(E) + q_a^j(E)$$
  
=  $\frac{\pi}{k^2} \sum_{l=0}^{l_{max}} (2l+1)[|1-S_l^j|^2 + (1-|S_l^j|^2)],$  (6)

where  $q_e^j(E)$  and  $q_a^j(E)$  are elastic and absorption cross sections, respectively,  $S_l^j$  is the *l*th complex scattering matrix element of the *j*th atom, which is related to the partial-wave phase shift as  $S_{i}^{J} = \exp(2i\delta_{i})$ . To obtain  $S_{i}^{J}$ , we solve the following radial equation:

 $i(\mathbf{n})$ 

$$\left(\frac{d^2}{dr^2} + k^2 - 2V_{opt}(r,k) - \frac{l(l+1)}{r^2}\right)u_l(r) = 0, \quad (7)$$

under the boundary condition

 $i(\mathbf{n})$ 

$$u_l(kr) \sim kr[j_l(kr) - in_l(kr)] + S_lkr[j_l(kr) + in_l(kr)],$$
(8)

where  $j_l$  and  $n_l$  are Spherical Bessel and Neumann functions separately.

In the present investigation, the atoms of a molecule are replaced by the appropriate complex optical potential

$$V_{opt}(r) = V_s(r) + V_e(r) + V_p(r) + V_a(r).$$
(9)

Thus  $V_{opt}(r)$  incorporates all the important physical effects. Presently, the static potential  $V_s(r)$  for *e*-atom systems is calculated by using the atomic charge density, determined from the well-known Hartree-Fock atomic wave functions [24]. The exchange potential  $V_e(r)$  provides a semiclassical energy-dependent form of Truhlar and co-workers [25],

$$V_e(r) = -\frac{1}{4} \left[ \sqrt{(k^2 - 2V_s)^2 + 16\pi\rho_0} - (k^2 - 2V_s) \right],$$
(10)

where  $k^2$  and  $\rho_0$  are the energy of incident electron and atomic-charge-density, respectively.

Zhang et al. [26] give a smooth form at all r for the polarization potential  $[V_n(r)]$ , which has a correct asymptotic form  $-\alpha/2r^4$  at large r and approaches the free-electron-gas correlation energy  $V_{ca}(r)$  proposed by Perdew and Zunger [27] in the near-target region

$$V_p(r) = -\frac{\alpha}{2(r^2 + r_{co}^2)^2},$$
(11)

where the constant  $r_{co}$  can be determined by letting  $V_p(0)$  $= -\alpha/2r_{co}^4 = V_{co}(r=0)$  and  $\alpha$  is the atomic polarizability. This potential model has been proved to be fairly successful in obtaining the TCS for electron-atom scattering [26].

The imaginary part of the optical potential  $V_a$  is the absorption potential, which represents approximately the combined effect of all the inelastic channels. Here we employ a semiempirical absorption potential as discussed by Staszewska et al. [28]. The  $V_a$  is a function of atomic charge density, incident electron energy, and mean excitation energy  $\Delta$  of the target. It is written as [28]



FIG. 1. Total cross sections for  $E - C_2F_4$  scattering. Solid curve, the EGAR results; broken curve, the 100% AR.

$$V_{a}(r) = -\rho(r)(T_{L}/2)^{1/2}(8\pi/5k^{2}k_{f}^{3})$$
$$\times H(k^{2} - k_{f}^{2} - 2\Delta)(A + B + C), \qquad (12)$$

where

$$\begin{split} T_L &= k^2 - V_s - V_e - V_p \,, \\ A &= 5k_f^3/2\Delta \,, \\ B &= -k_f^3(5k^2 - 3k_f^3)/(k^2 - k_f^2)^2 \,, \\ C &= 2H(2k_f^2 + 2\Delta - k^2) \frac{(2k_f^2 + 2\Delta - k^2)^{5/2}}{(k^2 - k_f^2)^2} \,, \end{split}$$

and  $k_f$  is the Fermi momentum. Here H(x) is a Heaviside function defined by H(x)=1, for  $x \ge 0$  and H(x)=0 for x < 0. The absorption potential  $(V_a)$  has been employed widely to calculate inelastic cross sections for *e*-atom [29] scattering.



FIG. 2. Total cross sections for  $E - C_2F_6$  scattering. Solid curve, the EGAR results; broken curve, the 100% AR. The experimental data:  $\bullet$ , Ref. [19].



FIG. 3. Total cross sections for  $E - C_3F_6$  scattering. Solid curve, the EGAR results; broken curve, the 100% AR.

### **III. RESULTS AND DISCUSSIONS**

Using the present optical potential, we have obtained qualitatively good TCS results for electron scattering by Ar, Kr, Xe [29] and Na [30] compared with many experimental data. At intermediate and high energies, our results are within experimental error. The e-atom potentials employed in this work appear to be satisfactory, at least for the calculation of the TCS on atoms in the present energy range. In this paper, employing the 100% additivity rule (AR) [Eq. (1)] and the energy-dependent geometric additivity rule (EGAR) [Eq. (2)], we have obtained the TCS for electron scattering from C<sub>2</sub>F<sub>4</sub>, C<sub>2</sub>F<sub>6</sub>, C<sub>3</sub>F<sub>6</sub>, C<sub>3</sub>F<sub>8</sub>, C<sub>6</sub>F<sub>6</sub>, and C<sub>6</sub>H<sub>6</sub> molecules in 30-3000 eV. The TCSs for H, C, F atoms have been given employing optical potential method in reference [15]. The present results on molecules are reported in Table I at selected collision energies and are plotted within the background of available experimental data [19–23] in Figs. 1-6. No other theoretical calculations for the TCS on all these molecules are found in the present energy region concerned.

In Fig. 1 for  $C_2F_4$  molecule and Fig. 3 for the  $C_3F_6$  molecule, the two present theoretical results are presented with-



FIG. 4. Total cross sections for  $E - C_3F_8$  scattering. Solid curve, the EGAR results; broken curve, the 100% AR. The experimental data:  $\bullet$ , Ref. [23].



FIG. 5. Total cross sections for  $E - C_6F_6$  scattering. Solid curve, the EGAR results; broken curve, the 100% AR. The experimental data:  $\bullet$ , Ref. [20].

out any available experiments and theories for comparison. The EGAR results are about 20.5-0.9%, for  $C_2F_4$ , and 31.4-1.2%, for  $C_3F_6$ , lower than these of the 100% AR in 30-3000 eV, and they merge well at higher energies. The discrepancy between results is higher for  $C_3F_6$  than for  $C_2F_4$  molecules, which indicates a larger contribution for the shielding effect in the  $C_3F_6$  molecule. Figures 2 and 4 show that our EGAR calculations on  $C_2F_6$  and  $C_3F_6$  molecules and corresponding experimental measurements [19,23] are in perfect agreement at the entire overlap of energies. For  $C_3F_6$ , the present EGAR results are about 15% higher than experimental data. On the other hand, compared with the EGAR results in these two figures, the 100% AR results are high and agree well with the EGAR results at high energies.

For the  $C_6F_6$  molecule, Szmytkowski and co-workers [19] have recently completed the measurements for TCS in *E* (250 eV, and their results and our calculations are shown in Fig. 5. Figure 5 shows, at all overlapped energies, that the present two results merge well with experimental measurements. Our results of the EGAR approach, which are about 0.9–33.3% lower than the calculation in the AR approach and about 6.2–48.7% higher than the experimental data at all



FIG. 6. Total cross sections for  $E - C_6H_6$  scattering. Solid curve, the EGAR results; broken curve, the 100% AR. The experimental data:  $\bullet$ , Ref. [21];  $\Box$ , Ref. [22].

overlapped energies, show better results than those of the 100% AR approach. No experimental data are found in the higher-energy region. But we promise that the present EGAR results will be good at E > 400 eV, which can also be noticed from Figs. 2, 4, and 6. For C<sub>6</sub>F<sub>6</sub> in Fig. 5 and for C<sub>6</sub>H<sub>6</sub> in Fig. 6, we find a good general accord between these two approaches in the limit of high energy (>1000 eV). The results of the EGAR are closer to the experimental TCS than those of the 100% AR in the present energy region. On the  $C_6H_6$  molecule, two groups of measurements are plotted in Fig. 6 and show some discrepancy, particularly in lower collision energy. Our EGAR and 100% AR results are about 18.8-60.2 % and 21.9-98.8 % higher than the measurements of Zecca and coworkers in 30-500 eV, respectively. Here, the results show that our calculations in EGAR and the 100% AR approaches present a larger discrepancy against experimental measurements at low and intermediate energies. The discrepancy results from, in the low- and intermediate-energy range, a large contribution of the three C=C bonding in the  $C_6H_6$  molecule. As the collision energy increases, the calculations and the measurements are in good agreement.

In general, both our theories exceed experimental values in the low- and intermediate-energy region, but the EGAR approach fares better. Since the contribution from the interference occurring between the scattering amplitudes originating from the different constituent atoms of the molecule is not included in the two additivity approaches, the TCSs obtained show larger discrepancies compared with the experimental data at low and intermediate energies. In the highenergy region, the present two results are in agreement with experimental measurements and show that the additivity rule is viable for complex polyatomic molecules. For our results, we assume that the errors are caused mainly by the additivity model at low energies. At intermediate and high energies, the present approaches and optical potential are a good approach and the errors caused by them are within the experimental errors. Employing the EGAR, we obtain the TCS on other molecules (CO<sub>2</sub>, NH<sub>3</sub>, SF<sub>6</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>3</sub>H<sub>6</sub>, C<sub>4</sub>H<sub>10</sub>, etc.) and the results are in better agreement with available experiments than the 100% AR results in Refs. [17,18].

In this paper, the 100% AR and EGAR have been introduced with the aim of generating reliably the TCS for electron scattering from complex polyatomic molecules ( $C_2F_4$ ,  $C_2F_6$ ,  $C_3F_6$ ,  $C_3F_8$ ,  $C_6F_6$ , and  $C_6H_6$ ) in the intermediateand high-energy region. Considering semiempirically geometric shielding effects in molecules, the modified AR, depending on molecular properties without any adjusted parameters, is simple but more effective when compared with available experimental data. It presents better results for the TCS on complex molecules  $C_2F_6$ ,  $C_3F_8$ ,  $C_6F_6$ , and  $C_6H_6$ . Although there are no other experiments and theories for comparison, we think, for  $C_2F_4$ ,  $C_3F_6$ , that the present EGAR results on the TCS are reliable, particularly in the high energy region. In view of a lot of samples, the EGAR and the optical potential model of related atoms can be used successfully to calculate qualitatively the TCS for e-polyatomic molecule scattering in intermediate- and highenergy ranges. The modified additivity rule (2) and the 100%

additivity rule give an interesting model for the TCS of electron scattering from polyatomic molecules and are of value for further research. Despite the fact that the mathematical calculations are not exact, the present results provide a good qualitative comparison and will be useful in experimental research, particularly for complex polyatomic molecules for which other exact calculations are difficult. In the meantime, we also hope to see that more and more theoretical and ex-

perimental research for the TCS on  $C_2F_4$ ,  $C_2F_6$ ,  $C_3F_6$ ,  $C_3F_6$ ,  $C_3F_8$ ,  $C_6F_6$ , and  $C_6H_6$  molecules is completed at intermediate and high energies in the near future.

### ACKNOWLEDGMENT

This work is supported by Henan Natural Science Foundation and Henan Education Foundation.

- L.G. Christophorou, *Electron Molecule Interactions and Their* Applications (Academic, New York, 1984).
- [2] O. Sueoka, S. Mori, and A. Hamada, J. Phys. B 27, 1453 (1994).
- [3] A. Zecca, J.C. Nogueira, G.P. Karwasz, R.S. Brusa, J. Phys. B 28, 477 (1995).
- [4] G. Garcia and F. Manero, Phys. Rev. A 53, 250 (1996).
- [5] Cz. Szmytkowski, G. Kasporski, and P. Mozejko, J. Phys. B 28, L629 (1995).
- [6] T.D. Mark and G.H. Dunn, *Electron Impact Ionization* (Springer, New York, 1985).
- [7] M. Bobeldijk, W.J. van der Zande, and P. G. Kistemaker, Chem. Phys. **179**, 125 (1994).
- [8] K.J. Miller, J. Am. Chem. Soc. 112, 8533 (1990).
- [9] J.F. Sun, G.Q. Yu, Y.H. Jiang, and S. Zhang, Eur. Phys. J. D 4, 83 (1998).
- [10] H. Deutsch, K. Becker, J. Pittner, V.B. Koutecky, S. Matt, and J.D. Mark, J. Phys. B 29, 5175 (1996).
- [11] D. Raj, Phys. Lett. A 160, 571 (1991).
- [12] K.N. Joshipura and P.M. Patel, Z. Phys. D: At., Mol. Clusters 29, 269 (1994).
- [13] J.F. Sun, Y.H. Jiang, and L.D. Wan, Phys. Lett. A 195, 81 (1994).
- [14] Y.H. Jiang, J.F. Sun, and L.D. Wan, Z. Phys. D: At., Mol. Clusters 34, 29 (1995).
- [15] Y.H. Jiang, J.F. Sun, and L.D. Wan, Phys. Rev. A 52, 398 (1995).

- [16] K.N. Joshipura and P.M. Patel, J. Phys. B 29, 3925 (1996).
- [17] Y.H. Jiang, J.F. Sun, and L.D. Wan, Phys. Lett. A 237, 53 (1997).
- [18] Y.H. Jiang, J.F. Sun, and L.D. Wan, J. Phys. B 30, 5025 (1997).
- [19] Cz. Szmytkowski, P. Mozejko, G. Kasperski, and E. P. Denga, J. Phys. B 33, 15 (2000).
- [20] Gr. Kasperski, P. Mozejko, and Cz. Szmytkowski, Z. Phys. D: At., Mol. Clusters 42, 187 (1997).
- [21] P. Mozejko, Gr. Kasperski, Cz. Szmytkowski, Gr.P. Karwasz, R.S. Brusa, and A. Zecca, Chem. Phys. Lett. 257, 309 (1996).
- [22] O. Sueoka, J. Phys. B 21, L631 (1988).
- [23] H. Tanaka, Y. Tachibana, M. Kitajima, O. Sueoka, H. Takaki, A. Hamada, and M. Kimura, Phys. Rev. A 59, 2006 (1999).
- [24] E. Clementi and C. Roetti, At. Data Nucl. Data Tables 14, 177 (1974).
- [25] M.E. Riley and D.G. Truhlar, J. Chem. Phys. 63, 2182 (1975).
- [26] X.Z. Zhang, J.F. Sun, and Y.F. Liu, J. Phys. B 25, 1893 (1992).
- [27] J.P. Perdew and A. Zunger, Phys. Rev. B 23, 5048 (1981).
- [28] G. Staszewska, D.W. Schwenke, D. Thirumalai, and D.G. Truhlar, Phys. Rev. A 28, 2740 (1983).
- [29] Y.H. Jiang, J.F. Sun, and L.D. Wan, Chin. J. At. and Mol. Phys. 11, 418 (1994).
- [30] J.F. Sun, Y.H. Jiang, and L.D. Wan, Chin. J. At. and Mol. Phys. 12, 56 (1995).