Vol 17 No 6, June 2008
1674-1056/2008/17(06)/2103-07

Chinese Physics B

© 2008 Chin. Phys. Soc.
and IOP Publishing Ltd

Additivity rule for electron–molecule total cross section calculations at 50–5000 eV: a new geometrical approach*

Shi De-Heng(施德恒)†, Sun Jin-Feng(孙金锋), Zhu Zun-Lüe(朱遵略), and Liu Yu-Fang(刘玉芳)

College of Physics and Information Engineering, Henan Normal University, Xinxiang 453007, *China*

(Received 10 October 2007; revised manuscript received 9 November 2007)

Taking into consideration the changes of the geometric shielding effect in a molecule as the energy of incident electrons varies, this paper presents an empirical fraction, which depends on the energy of incident electrons, the target's molecular dimension and the atomic and electronic numbers in the molecule. Using this empirical fraction, it proposes a new formulation of the additivity rule. Employing the new additivity rule, it calculates the total cross sections of electron scattering by C_2H_4, C_6H_6, C_6H_{14} and C_8H_{18} over the energy range from 50 to 5000 eV. In order to exclude the calculation deviations caused by solving the radial Schrödinger equation of electron scattering by atoms, here the atomic cross sections are derived from the experimental total cross section results of simple molecules (H_2, O_2, CO) via the inversion algorithm. The quantitative total cross sections are compared with those obtained by experiments and other theories, and good agreement is obtained over a wide energy range, even at energy of several tens of eV.

Keywords: electron scattering, total cross section, additivity rule, geometric shielding effect
PACC: 3480

1. Introduction

Total cross section (TCS) for electron scattering by molecules plays a central role in many fields. Nevertheless there is a lack of accurate theoretical approaches at intermediate and high energies at which almost all molecular inelastic channels (rotational, vibrational, electronic excitation and ionization process, etc) are open. Consequently, to obtain the accurate TCSs for electron scattering by molecules at higher energies, many new approximation methods have been proposed and developed in the past years of several tens. Of these methods, the additivity rule (AR) model[1] is a fairly simple and practical one, particularly for simpler and smaller molecules at high enough energies. But for complex molecules,[2,3] great discrepancies still exist even at energy of several hundreds of eV.

In order to extend the AR model validity to lower energies, some investigations have been made in recent years. Bobeldijk *et al*[4] have presented two geometric AR (GAR) methods, and obtained encouraging electron impact ionization cross section (ICS) of several molecules at energy of several tens of eV, but they did not calculate the TCSs of electron scattering by molecules. Deutsch *et al*[5] have applied a modified AR (with an atomic weighted factor) to the molecular ICS, but they too did not calculate the molecular TCS. Zecca *et al*[6] have proposed a new AR formula, which takes into account the geometrical screening of the component atoms in a molecule. Using this formula, they have evaluated the TCSs of electron scattering by NO, N_2O, CO_2, NO_2 and CH_4. Favourable agreement with measurements is obtained at intermediate and high energies. However, as pointed out by Blanco and García,[7] this approach is very complicated for complex molecules. To simply compute the molecular TCS, Blanco and García[7,8] have put forward a modification method named the screen corrected AR (SCAR) procedure, which takes into consideration the geometrical screening corrections due to mutual screening of atoms inside a molecule. And their results from application of such method to N_2, CO, CO_2 and C_6H_6 show an appreciable improvement in the 10 to 1000 eV region. Karwasz *et al*[9] proposed a formation of the AR, where a molecular cross section can be approximated by a Born-like two-parameter formula. Though this method can attain good results over a wide energy range, the applications are limited since the two adjustable values are

*Project supported by the National Natural Science Foundation of China (Grant No 10574039) and the Program for Science and Technology Innovation Talents in Universities of Henan Province in China (Grant No 2008HASTIT008).
†E-mail: scattering@sina.com.cn

different for each target, and their value determinations require experimental findings. Recently, finding the TCSs of electron scattering by molecules, Antony *et al*[10] have also presented a modified AR named the group additivity method, where the cross section arising from each constituent group of a molecule was added together to obtain the molecular TCS. Using this method, they have computed the TCSs of electron scattering by several molecules. Good agreement with experiments is attained over a wide energy range. Jiang *et al*[11] have put forward a modification method named the energy-dependent geometric AR (EGAR) approach, and evaluated the TCSs for electron scattering by a number of molecules. Since the target's molecular dimension is not considered, obvious deviations still exist at lower energies for complex molecules. To improve the agreement between theory and experiment, very recently, we take into consideration the shielding effect of atoms in the molecule and introduce a further modification to the EGAR model, which is dependent on the target's molecular dimension, the energy of incident electrons and the total atomic and electronic numbers in the molecule.

Considering the changes of the geometric shielding effect in a molecule as the energy varies, this paper presents an empirical fraction, which depends on the molecular specifications and the energy. The modified AR model is used to calculate the TCSs of electron scattering by a relatively smaller molecule (C_2H_4) and three relatively larger ones (C_6H_6, C_6H_{14} and C_8H_{18}) at 50–5000 eV. In order to exclude the calculation deviations caused by solving the radial Schrödinger equation of electron scattering by atoms, in this paper, the atomic cross sections are derived from the experimental TCS results of simple molecules (H_2, O_2, CO). In Section 2, we describe in detail the present modified AR model. In Section 3, we present the TCSs, compare them with available experimental and other theoretical results and make some necessary discussion. And in Section 4, conclusions are made. Atomic units are used throughout this paper otherwise specified.

2. Theory and method

Assuming that each atom in a molecule scatters independently and that redistribution of atomic electrons due to the molecular binding is unimportant, we can reduce the electron–molecule collision into the problem of collision with individual atoms. Consequently the following AR model can be obtained:

$$Q_{\mathrm{AR}}(E) = \sum_{j=1}^{N} q_{\mathrm{T}}^{j}(E). \tag{1}$$

Where $q_{\mathrm{T}}^{j}(E)$ denotes the TCS of electron scattering by the jth constituent atom. In Eq.(1), one main effect is not considered: a close-packed molecule is not fully transparent for low-energy electrons, and the "inner" atoms are partially shielded by the "outer" atoms and contribute less to the molecular TCS at lower energies than those at higher energies. The shielding effect, which leads to negative contributions to the TCS in the original AR model, is dependent on the molecular geometry. Accounting for the shielding effect, Bobeldijk *et al*[4] have introduced the GAR model to evaluate the molecular ICS. We find that the GAR model, which incorporates the geometrical shielding effect in a molecule, is a good approach to obtain the molecular TCS, particularly for complex molecules at low energies.[11] When the GAR model is applied to calculate the molecular TCS, it can be expressed as

$$Q_{\mathrm{GAR}}(E) = \frac{1}{3}Q_{\parallel}(E) + \frac{2}{3}Q_{\perp}(E), \tag{2}$$

where, $Q_{\parallel}(E)$ and $Q_{\perp}(E)$ are the TCS for electron approaching the molecule parallel to the Z axis ($\theta = 0^{\circ}$) and the TCS for an approach perpendicular to the Z axis ($\theta = 90^{\circ}$), respectively. Here, the coordinate system is fixed to the centre of the molecule and the Z-axis is attached to its longest symmetrical axis. For instance, in the case of C_2H_4, C_6H_6, C_6H_{14} and C_8H_{18}, $Q_{\parallel}(E)$ and $Q_{\perp}(E)$ equal $Q_{\mathrm{CH_2}}$, $3Q_{\mathrm{C_2H}}$, $Q_{\mathrm{CH_3}}$, $Q_{\mathrm{CH_3}}$ and $2Q_{\mathrm{CH_2}}$, $3Q_{\mathrm{CH}}$, $6Q_{\mathrm{CH_2}}$, $8Q_{\mathrm{CH_2}}$, respectively. More precisely, $Q_{\mathrm{CH_2}}$, $Q_{\mathrm{C_2H}}$, Q_{CH} and $Q_{\mathrm{CH_3}}$ are the TCSs of electron scattering by CH_2, C_2H, CH and CH_3, respectively, and still obtained by the original AR model.

Calculations have shown that the GAR model is valid at lower energies[11] and overestimates the shielding effect in molecules over the high-energy range, resulting in lower TCS results. In comparison, the AR model is accurate at high enough energies[2,3] and disregards the shielding effect over the low-energy range, resulting in higher TCS results when compared with experiments, especially for complex molecules. We know that a close-packed molecule is not fully transparent for low-energy electrons, but the transparency will increase with the energy of incident electrons. That is to say, when the energy is very low, the "inner"

atoms are shielded partially by the "outer" atoms, thus the GAR model can give favourable TCS results, but the AR model not. When the energy is high enough, the molecule is fully transparent and each atom in the molecule scatters independently. Thus the interaction effect between atoms can be neglected at sufficiently high energies. Hence, the AR model is valid, but the GAR model not. Taking into account these factors, we incorporate the advantages of the GAR and AR models, and present the following AR formula,

$$Q_{\mathrm{TCS}}(E) = Q_{\mathrm{GAR}}(E) + A[Q_{\mathrm{AR}}(E) - Q_{\mathrm{GAR}}(E)]. \quad (3)$$

Here, A is an empirical fraction, which signifies the contribution of shielded atoms for different molecules at different energies. Now, the key problem is how to determine the empirical fraction A so as to correctly reflect the changes of the geometric shielding effect in the molecule as the energy of incident electrons varies. To determine the parameter A, Jiang *et al*[11] thought that three factors should be taken into account. Firstly, when the energy is low enough, since the GAR model is valid, the value of A must satisfy $Q_{\mathrm{TCS}}(E) \approx Q_{\mathrm{GAR}}(E)$. And when the energy is high enough, because the AR model is accurate, A must satisfy $Q_{\mathrm{TCS}}(E) \approx Q_{\mathrm{AR}}(E)$. It means that the higher the energy is, the less effect geometrical shielding will have on the TCS of the molecule. Secondly, at the same energy, the more complex the molecule, the smaller is the A. And thirdly, the empirical fraction A should be related to the energy E and the total electronic number m in the molecule so as to ensure the reasonable shape for the TCS against experimental data over a wide energy range. According to these, Jiang *et al*[11] assumed that

$$A = \frac{E}{mC + E}. \quad (4)$$

Here, E is in units of eV and C is a constant, which equals to 1 eV.

Calculations have proved that Eq.(4) can give favourable TCSs for smaller or simpler molecules (such as H_2O, CO, CO_2, NO, NO_2 and N_2O). But for larger or more complex molecule (such as the molecules studied in this paper), it can still not ensure the reasonable shape of the TCS curve against experimental data over a wide energy range. This can be clearly seen in log–log curves plotted by using the TCSs calculated by it. The main problem is that these log–log curves are still steeper than those plotted by the corresponding experimental data. It suggests that the geometric shielding corrections in Eq.(4) are not enough at lower energies. Having checking the equation carefully, we find that it includes only one of the molecular specifications, the total electronic number m in the molecule. Other molecular specifications, such as the molecular geometric dimension and the total atomic number in the molecule, are excluded. Consequently for larger or more complex molecules, it cannot give favourable TCSs at lower energies. In order to obtain more accurate TCSs, we think that at least two additional factors should be considered. Firstly, at a given energy, we have found that the larger the size of a molecule, the greater is the discrepancy between the TCSs calculated by this equation and the experiments. It implies that the larger the volume of a molecule is, the smaller the empirical fraction A should be. Secondly, at a given energy, we have also found that when molecules have the same total electronic number, the greater the total atomic number in the molecule, the smaller the empirical fraction A should be. In accordance with above discussion, we assume that the empirical fraction A over the whole energy range behaves as

$$A = \frac{E}{mndC + E}. \quad (5)$$

Here, n is the atomic number in the molecule. d is the target's molecular dimension in atomic units, which can be roughly determined by the bond length and the bond angle.[12] And C is a constant considering the reasonable dimension relation, which equals to $1\,\mathrm{eV}/a_0$.

Is the problem, of which the log–log curves are steeper than those obtained by experiments, brought by the AR model itself, or by the theoretical calculations for electron-atom scattering? In order to exclude the theoretical calculation suspicion of electron-atom cross sections, here we use the inversion algorithm describing above [Eqs.(3) and (5)] to determine the atomic cross sections of electron scattering by C, O and H from the measured TCSs of H_2, O_2 and CO, which come from the Trento laboratory.[13−15] The derived atomic cross sections are tabulated in Table 1.

Table 1. TCSs in units of a_0^2 for electron scattering by atoms C, O and H.

E/eV	C	O	H	E/eV	C	O	H	E/eV	C	O	H
50	23.607	22.429	7.857	500	7.107	6.893	1.393	5000	0.893	0.893	0.254
100	19.179	18.179	5.250	1000	3.964	3.929	0.750				
200	13.714	13.000	3.071	2000	2.143	2.107	0.393				

3. Results and discussion

Using the present modified AR model and the atomic TCSs derived from the experiments, we have calculated the TCSs of electron scattering by a number of molecules. Good agreement with experiments is attained over a wide energy range, even at energy of several tens of eV for some of them. It shows that the present model [Eq.(5)] is the right dependence on the involved parameters. Here we in detail report the TCSs of electron scattering by C_2H_4, C_6H_6 (benzene), C_6H_{14} (normal hexane) and C_8H_{18} (normal octane) calculated by Eq.(5) (present modified AR results), the TCSs calculated by Eq.(1) (present unmodified AR results) and the TCSs calculated by Eq.(4) (original modified AR results). These results together with available experimental and other theoretical data are depicted in Figs.1–4, respectively.

For the TCSs of electron scattering by C_2H_4, we have found four groups of measurements obtained by Ariyasinghe and Powers[16] at 200–1400 eV, Sueoka and Mori[17] at 0.7–400 eV, Nishimura and Tawara[18] at 4–500 eV and Szmytkowski *et al*[19] at 0.6–370 eV, and three groups of theories given by Vinodkumar *et al*[20] at 50–2000 eV, Joshipura and Vinodkumar[21] at 50–5000 eV and Liu *et al*[22] at 10–5000 eV in the involving energy range. We depict the original modified AR results, the present modified and unmodified AR results, four groups of measurements[16−19] and one group of theoretical calculations given by Vinodkumar *et al*[20] in Fig.1. In order to avoid congestion, some results, such as the ones obtained by Joshipura and Vinodkumar[21] and the ones obtained by Liu *et al*,[22] are not included in Fig.1. In theories, the present modified AR results are in better agreement with the measurements[18,19] but in poorer accord with the ones[17] than the theories obtained by Vinodkumar *et al*[20] at intermediate and low energies. In experiments, the present modified AR results are in excellent agreement with all these measurements[16−19] at the whole overlapping energies except those obtained by Sueoka and Mori[17] below 200 eV. (It should be noticed that there are great differences between the measurements obtained by Sueoka and Mori[17] and the measurements obtained by Nishimura and Tawara[18] and Szmytkowski *et al*[19] at lower energies, especially below 100 eV). Nevertheless the original modified AR results show greater deviations than the present modified ones when compared with these measurements[16−19] at intermediate and low energies.

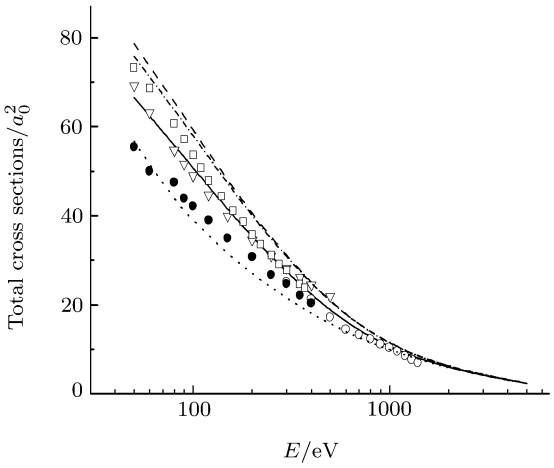


Fig.1. TCSs for electron–C_2H_4 scattering. Theoretical calculations: solid line, present modified AR results; short-dash-dotted line, original modified AR results; dashed line, present unmodified AR results; dotted line, Vinodkumar *et al*.[20] Experimental findings: open circle, Ariyasinghe and Powers;[16] full circle, Sueoka and Mori;[17] open triangle, Nishmura and Tawara;[18] open square, Szmytkowski *et al*.[19]

Figure 2 illustrates the original modified AR results, the present modified and unmodified AR results of electron scattering by C_6H_6 along with the measurements obtained by Makochekanwa *et al*[23] at 50–1000 eV, Sueoka[24] at 50–400 eV, the Trento group[25] at 90–3500 eV and the Gdansk group[25] at 50–250 eV. For the sake of clarity, a number of theoretical results, such as the ones obtained by Blanco and García[7] at 10–1000 eV, the ones obtained by Blanco and García[8] at 10–10000 eV and the ones obtained by Jiang *et al*[11] at 30–3000 eV, are omitted in Fig.2. Obviously, the present modified AR results are in excellent agreement with the measurements obtained by Makochekanwa *et al*,[23] the Trento group[25] and the Gdansk group[25] almost at all the overlapping energies, and also in good accord with the mea-

surements obtained by Sueoka[24] above 200 eV. (It should be pointed out that the experiments obtained by Sueoka[24] are much smaller than those obtained by others[23,25] at lower energies.) For example, the differences between the present modified AR results and the measurements obtained by the Trento group[25] are of only 8.6%, 2.6%, 0.3% and 1.3% at 100, 200, 500 and 2000 eV, respectively; and the differences between the present modified AR results and the measurements obtained by Makochekanwa *et al*[23] are of only 5.2%, 3.6% and 4.2% at 50 , 100 and 1000 eV, respectively, too. In contrast with the present modified AR results, the original modified and the present unmodified AR results show great deviations when compared with the measurements[23–25] at intermediate and low energies. Even compared with those obtained by Sueoka[24] below 200 eV, the present modified AR results are also obviously closer to them than the original modified and the present unmodified ones. Therefore, as a whole, for the proposed formula, good agreement with measurements is obtained when the energy of incident electrons is above 100 eV or so.

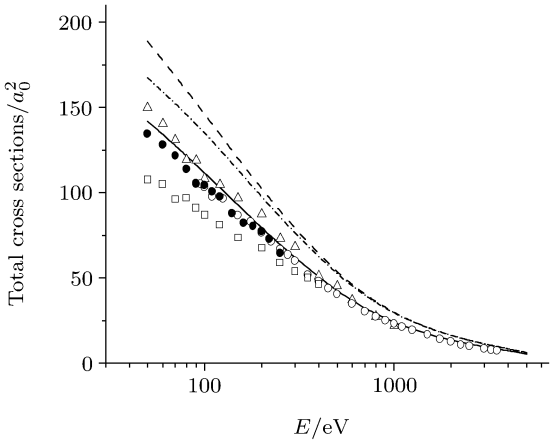


Fig.2. TCSs for electron–C_6H_6 scattering. Theoretical calculations: solid line, present modified AR results; short-dash-dotted line, original modified AR results; dashed line, present unmodified AR results. Experimental findings: open triangle, Makochekanwa *et al*;[23] open square, Sueoka;[24] open circle, the Trento group;[25] full circle, the Gdansk group.[25]

As far as the TCSs of electron scattering by C_6H_{14} is concerned, only group of measurements[26] at 0.4–1000 eV exists and no theoretical results are available for comparison in the present energy region. The original modified AR results, the present modified and unmodified AR results as well as the only measurements are shown in Fig.3. From Fig.3, one can clearly see that the present modified AR results are in excellent agreement with the only measurements at all the overlapping energies. Above 1000 eV, no experiments have been found elsewhere to this day. But according to the good agreement between the present modified AR results and the measurements, we conclude that the present modified AR results above 1000 eV are reliable and accurate.

In Fig.4 for electron–C_8H_{18} scattering, we report the comparison between the original modified AR results, the present modified and unmodified AR results and the only group of measurements obtained by Sueoka *et al.*[27] Obviously, good agreement can be found between the present modified AR results and the only measurements above 100 eV or so. As shown in Figs.3–4, the original modified and the present unmodified AR results are greatly higher than the measurements at intermediate and low energies.

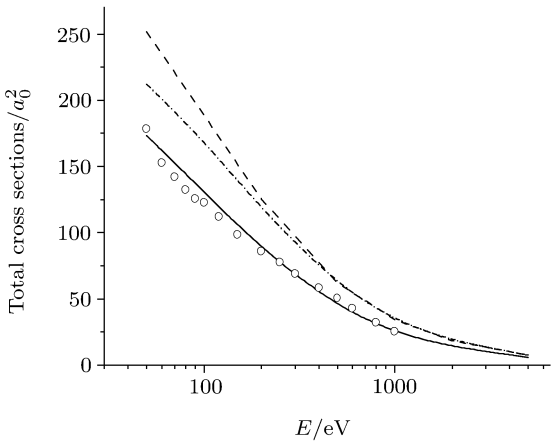


Fig.3. TCSs for electron–C_6H_{14} scattering. Theoretical calculations: solid line, present modified AR results; short-dash-dotted line, original modified AR results; dashed line, present unmodified AR results. Experimental findings: circle, Sueoka *et al.*[26]

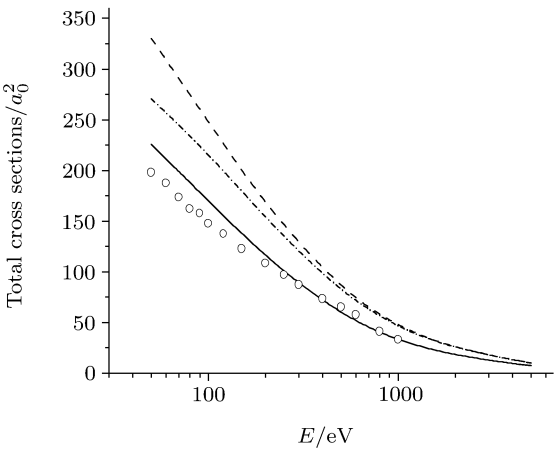


Fig.4. TCSs for electron–C_6H_{18} scattering. Theoretical calculations: solid line, present modified AR results; short-dash-dotted line, original modified AR results; dashed line, present unmodified AR results. Experimental findings: circle, Sueoka *et al.*[27]

At lower energies, as illustrated in Figs.1–4, the present modified AR results are higher than almost all the measurements because we do not consider the interference effect originating from each constituent group in the molecule.[10] This effect may be important at energy of several tens of eV since the de Broglie wavelength (For example, the de Broglie wavelength is 0.1369 nm when the energy of incident electrons is 80 eV) associated with the incident electrons will become comparable to the bond length of the molecule. (For instance, the C-H and C-C bond lengths in C_6H_6 are of 0.1101 and 0.1399 nm,[12] respectively.) Thus it might lead to an overestimation of the calculated TCSs.[10] In addition, the multiple scattering and valence-bond distortion[28,29] are also neglected in the present investigations. It will increase the possibility of multiple scattering when the de Broglie wavelength of incident electrons is comparable to the internuclear distance of the molecule at energy of several tens of eV. It is expected that the inclusion of multiple scattering effect at lower energies will reduce the TCSs by a significant amount.[28] The likely effect of the valence-bond distortion is also to reduce the cross sections.[29] So, though we have taken into consideration the geometric shielding effect in the molecule, TCS differences still exist between the present modified AR results and the experiments at lower energies.

With the increase of energy, the wavelength of incident electrons becomes smaller and smaller compared with the molecular bond length, and the interactions among the atoms become weaker and weaker, then the above-mentioned effects contribute less and less. Consequently the higher the energy is, the better the present modified AR results are. So, the present modified AR approach can attain excellent calculations, as verified in Figs.1–4.

4. Conclusions

Considering the geometric shielding effect in a molecule, this paper puts forward an empirical fraction, which depends on the target molecular specifications and the energy of incident electrons. Using this fraction, we successfully combine the advantages of the GAR and AR models and obtain more reliable TCSs of electron scattering by complex molecules (C_2H_4, C_6H_6, C_6H_{14} and C_8H_{18}) in the present energy range. Great success has been made at lower energies, especially above 100 eV, even though we ignore the interference effect originating from each constituent group, the multicentre scattering effect and the valence-bond distortion effect in the present work. In addition, for the present modified AR model, the problem, for which the TCS log–log curve is steeper than those obtained by experiments, almost disappears. But for the original AR model or the original EGAR approach, the more complex the molecule, the steeper is the TCS curve when compared with the corresponding experiments, as shown in Figs.1–4. Meanwhile, we have to stress that the accuracy of our results somewhat depend on the experimental errors presented in the starting data of measured molecular cross section. As the experimental accuracy improves, or as the result of electron scattering from atom is accurately calculated, the present modified AR model must give more reliable TCSs of electron scattering from complex molecules. As further investigation, we will use the modified AR approach to calculate the differential cross sections and the moment transfer cross sections[30,31] so as to further verify the validation of this model.

References

[1] Raj D 1991 *Phys. Lett.* A **160** 571

[2] Shi D H, Sun J F, Liu Y F, Ma H and Zhu Z L 2006 *Acta Phys. Sin.* **55** 4096 (in Chinese)

[3] Shi D H, Sun J F, Sun J F, Zhu Z L and Liu Y F 2005 *Chin. Phys.* **14** 120

[4] Bobeldijk M, van der Zande W J and Kistemaker P G 1994 *Chem. Phys.* **179** 125

[5] Deutsch H, Becker K and Märk T D 1997 *Int. J. Mass Spectrom. Ion Proc.* **167/168** 503

[6] Zecca A, Melissa R, Brusa R S and Karwasz G P 1999 *Phys. Lett.* A **257** 75

[7] Blanco F and García G 2003 *Phys. Lett.* A **317** 458

[8] Blanco F and García G 2007 *Phys. Lett.* A **360** 707

[9] Karwasz G P, Brusa S, Piazza A and Zecca A 1999 *Phys. Rev.* A **59** 1341

[10] Antony B K, Joshipura K N and Mason N J 2005 *J. Phys.* B **38** 189

[11] Jiang Y H, Sun J F and Wan L D 2000 *Phys. Rev.* A **62** 062712

[12] Lide D R 1994 *CRC Handbook of Chemistry and Physics* 74th edn (Boca Raton, FL: CRC Press)

[13] Karwasz G P, Brusa S A, Gasparoli A and Zecca A 1993 *Chem. Phys. Lett.* **211** 529

[14] Zecca A, Karwasz G P and Brusa S A 1996 *Rivista del Nuovo Cimento* **19** 1

[15] Zecca A, Karwasz G P and Brusa S A 1996 28$^{\text{th}}$ *European Group Atomic Spectr. Conf.* (Graz, Austria) *Europhys. Conf. Abstr.* D **20** 302
[16] Ariyasinghe W M and Powers D 2002 *Phys. Rev.* A **66** 052716
[17] Sueoka O and Mori S 1986 *J. Phys.* B **19** 4035
[18] Nishimura H and Tawara H 1991 *J. Phys.* B **24** L363
[19] Szmytkowski C, Kwitnewski S and Denga E P 2003 *Phys. Rev.* A **68** 032715
[20] Vinodkumar M, Joshipura K N, Limbachiya C G and Antony B K 2006 *Eur. Phys. J.* D **37** 67
[21] Joshipura K N and Vinodkumar M 1999 *Eur. Phys. J.* D **5** 229
[22] Liu Y F, Shi D H, Sun J F, Zhu Z L and Yang X D 2005 *Commun. Theor. Phys.* **43** 309
[23] Makochekanwa C, Sueoka O and Kimura M 2003 *Phys. Rev.* A **68** 032707
[24] Sueoka O 1988 *J. Phys.* B **21** L631
[25] Moiejko P, Kasperski G, Szmytkowski C, Karwasz G P, Brusa R S and Zecca A 1996 *Chem. Phys. Lett.* **257** 309
[26] Sueoka O, Makochekanwa C, Tanino H and Kimura M 2005 *Phys. Rev.* A **72** 042705
[27] Sueoka O, Makochekanwa C and Kimura M 2006 *Eur. Phys. J.* D **37** 377
[28] Hayashi S and Kuchitsu K 1976 *Chem. Phys. Lett.* **41** 575
[29] Bonham R A and Iijima T 1963 *J. Phys. Chem.* **67** 2266
[30] Shi D H, Sun J F, Zhu Z L, Yang X D, Liu Y F and Ma H 2007 *Acta Phys. Sin.* **56** 4435 (in Chinese)
[31] Shi D H, Sun J F, Zhu Z L, Ma H, Liu Y F and Yang X D 2007 *Chin. Phys.* **16** 1655