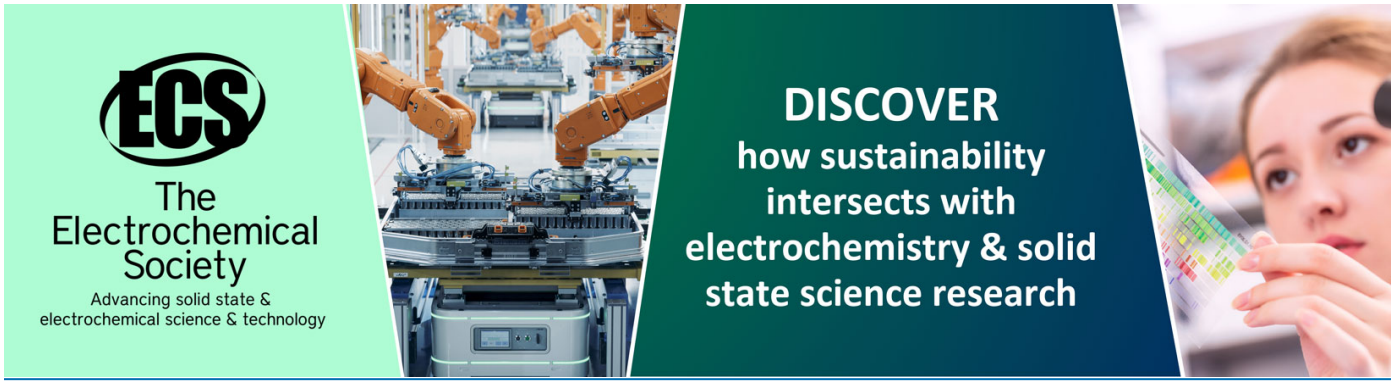
Calculation of (e, 2e) triple differential cross sections of Mg in coplanar geometry



Journal of Physics: Conference Series **288** (2011) 012008 doi:10.1088/1742-6596/288/1/012008

Calculation of (e, 2e) triple differential cross sections of Mg in coplanar geometry

G. Purohit*, Vinod Patidar and K. K. Sud

Department of Physics, School of Engineering, Sir Padampat Singhania University, Bhatewar, Udaipur-313 601, India

*g_vpurohit@yahoo.com, ghanshyam.purohit@spsu.ac.in

Abstract. We report the results of triple differential cross section of coplanar (e, 2e) processes on Mg (3s) atom in modified distorted wave Born approximation (DWBA). The standard DWBA formalism has been modified by including the correlation-polarization potential (which is function of electron density) and post collision interaction. We compare our computed results with the available experimental data and observe that the inclusion of polarization potential in the standard DWBA is able to improve the agreement with experimental results.

1. Introduction

Study of electron-impact single ionization (i.e. (e, 2e) processes) of atoms and ions provides important information about target structure, target wavefunction and collision dynamics. Since the experiment of Ehrhardt et al. [1] extensive studies have been performed for the electron impact single ionization of hydrogen [2] and helium [3] atoms in different geometrical arrangements. Apart from hydrogen and helium atoms, (e, 2e) studies have been performed on a number of targets using different theoretical approaches (see review articles [4-8]). There has been recent focus on the study of (e, 2e) process in coplanar symmetric geometry in which the incident and outgoing electrons lie in the same plane. We get a close insight of the (e, 2e) reaction in coplanar symmetric geometry due to clean knockout of the target electron. The symmetric collisions in which both the final state electrons have the same energy and are observed at the same scattering angles on opposite sides of the beam direction in the scattering plane, provide a severe test of the theory. Distorted wave Born approximation (DWBA) [9, 10] and convergent close coupling approximation (CCC) [11-13] have successfully described the salient features of the TDCS of hydrogen and helium atoms. There has been particular interest for the study of (e, 2e) processes in the low incident energy regime in coplanar symmetric geometry [11, 14]. The CCC approximation has been widely successful to explain the features of TDCS, however still there are certain discrepancies [15]. The extended complex scaling method [2] provides an exact framework for solving ionization problems. The time dependent close coupling (TDCC) formalism has been applied to study electron impact ionization of atoms [16-18]. TDCC has been used to investigate the fully differential cross section of He atom at incident electron energy 44.6 eV [17] and good agreement is found between experiment and TDCC results. However, there are certain discrepancies in the coplanar symmetric geometry.

The distorted wave Born approximation (DWBA) is well known and able to produce correct trends of TDCS for a wide variety of atomic targets above incident electron energy 50 eV [8]. For the (e, 2e) processes at low energies different physical effects are very important such as post-collision

interaction (PCI), charge cloud polarization, electron exchange etc. and these processes are responsible for the discrepancies between theory and experiment. Biava et al [19] have performed DWBA calculations of TDCS using different exchange effects and concluded that the exchange effects are particularly important for inner-valence ionization. Further improvement of the agreement between experiment and theory of the TDCS at low energy (e, 2e) processes can be achieved by proper treatment of PCI and inclusion of polarization [20, 21]. Various studies [22-26] have shown that inclusion of PCI and polarization potential in DWBA calculations improves the agreement of calculations with the experimental results significantly.

There has been recent focus on the study of (e, 2e) processes on alkali and alkali earth targets initiated by the experimental study of (e, 2e) processes in coplanar geometry by Murray and Cvejanovic [27] and Murray [28] on alkali and alkali earth targets Na, K and Mg, Ca. Study of (e, 2e) processes on these targets is of prime importance since these are having one and two electrons respectively in the valence shell and after ionization they are left as inert core (alkali target) and one electron in the valence shell above inert core (alkali earth target). Following the experimental results of Murray [28] several theoretical results have been reported for the (e, 2e) processes in coplanar geometry on the alkali and alkali earth targets [22, 29-34] and particularly, the study of (e, 2e) processes on Ca atom [22, 29, 32, 33]. Apart from the above mentioned studies Bolognesi et al. [35, 36] have reported a series of (e, 2e) measurements in unequal energy sharing conditions for the ionization of Mg (3s) target. Most of these studies have been performed in DWBA formalism and the first CCC calculation has been reported for the electron-sodium ionization in coplanar symmetric geometry [31]. We report the results of our modified distorted wave Born approximation calculations (DWBACPE) for Mg (3s) atoms. We modify the standard DWBA formalism by inclusion of correlation-polarization potential (as a function of electron density) and post collision interaction. We compare the results of TDCS with the recent available measurements of Murray [28].

2. Theory

The triple differential cross section for (e, 2e) process on a target may be written as

$$\frac{d^3\sigma}{d\Omega_1\, d\Omega_2\, dE_1} = (2\pi)^4 \frac{k_1 k_2}{k_0} \sum_{av} \left|T(k_1, k_2, k_0)\right|^2 \tag{1}$$

with

$$T(k_1, k_2, k_0) = \left\langle k_1 k_2 \left| T \right| \psi_{nl} k_0 \right\rangle .$$

The expression in Eq. (1) includes a sum over final and average over initial magnetic and spin state degeneracy. The T matrix in Eq.(1) is the reaction amplitude, it couples the initial states ψ_i and the final states. T includes interaction between the incident and target electrons and the nucleus. It is the part of the TDCS that is the subject of approximation. The T-matrix element which represent the ionization amplitude is conveniently written in terms of distorted waves as

$$\left\langle k_1 k_2 \left| T \right| \psi_{nl} k_o \right\rangle = \left\langle X_1^{(-)}(k_1)\, X_2^{(-)}(k_2) \right| v_1 + v_3 - U \left| \psi_i\, X_0^{(+)}(k_0) \right\rangle \tag{2}$$

The electron-electron potential v_3 is responsible for ionization and U is the distorting potential. Use of orthogonality between orbital ψ_i and distorted wave for ejected electron eliminates v_1 and U from the expression of T matrix element. As mentioned earlier the initial state ψ_i contains an electron bound to the atom core with separation energy E_b. The distorted waves for the incident and scattered electrons, $X_0^{(+)}(k_0)$ and $X_1^{(-)}(k_1)$, respectively, are calculated in a potential $U = \left\langle \psi_i \left| v_1 + v_3 \right| \psi_i \right\rangle$.

Equation (1) in terms of direct and exchange amplitudes may be written as

$$\frac{d^3\sigma}{d\Omega_1\, d\Omega_2\, dE_1} = (2\pi)^4 \frac{k_1 k_2}{k_0} \sum_{av} \left(|f|^2 + |g|^2 - \mathrm{Re}\left(f^* g\right) \right) \tag{3}$$

where

$$f = \left\langle X_1^{(-)}(k_1, r_1)\, X_2^{(-)}(k_2, r_2) \left| v_3 \right| X_0^{(+)}(k_0, r_1)\, \psi_{nl}(r_2) \right\rangle, \tag{4}$$

$$g = \left\langle X_1^{(-)}(k_1, r_2)\, X_2^{(-)}(k_2, r_1) \left| v_3 \right| X_0^{(+)}(k_0, r_1)\, \psi_{nl}(r_2) \right\rangle \tag{5}$$

here $v_3 = \frac{1}{|r_1 - r_2|}$ is the interaction potential between the incident and target electrons responsible for the ionization, $X_0^{(+)}$ is the distorted wavefunction for the incident electron, $X_1^{(-)}$ and $X_2^{(-)}$ represent the distorted wavefunctions for the two outgoing electrons and each is orthogonalized with respect to ψ_{nl}. Equations (4) and (5) are direct and exchange amplitudes for ionization from the (n, l) shell of the target atom where ψ_{nl} is the corresponding target orbital from which ionization is taking place and n and l are the principal and orbital quantum number respectively. We have used Hartree-Fock orbitals of Clementi and Roetti [37] for ψ_{nl}. The distorted wavefunction for the incident electron is generated in the equivalent local ground state potential of the atom whereas the distorted wavefunctions for the outgoing electrons are generated in the equivalent local ground state potential of the ion. For the work reported here we have made a careful check to ensure that the cross sections converge satisfactorily. The spin-averaged static-exchange potential [38] as modified by Riley and Truhlar [39] with the exchange potential taken in the equivalent local approximation is given as

$$V_E(r) = 0.5[E_0 + V_D(r) - \{[E_0 + V_D(r)]^2 - 2\pi\rho(r)^2\}^{1/2}] \tag{6}$$

where $\rho(r)$ is the electron density. The direct distorting potential $V_D(r)$ for the incident electron is obtained from the target radial orbital $u_{nl}(r)$ [40] as

$$V_D(r) = -\frac{Z}{r} + \sum_{nl} N_{nl} \int dr' [u_{nl}(r')]^2 / r_>, \tag{7}$$

where $r_>$ is the greater of r and r'. The details about the integration of the radial matrix element are described by McCarthy [40] and we have not given here for brevity. The equivalent local ground state potential V_{00}, which is the distorting potential, is the sum of exchange and direct potentials and is expressed as follows;

$$U = V_D(r) + V_E(r), \tag{8}$$

$$U = V_D(r) + 0.5[E_0 + V_D(r) - \{[E_0 + V_D(r)]^2 - 2\pi\rho(r)^2\}^{1/2}]. \tag{9}$$

We have modified the distorting potential (eq. (9)) used to calculate distorted waves $X_0^{(+)}$, $X_1^{(-)}$ and $X_2^{(-)}$ by addition of correlation-polarization potential V_{CP} to see the effect of electron correlation and target polarization on the trend of TDCS (DWBACPE calculations). The fundamental form of the short range correlation plus long range polarization potential may be approximated by means of local density functional theory (Padial and Norcross [41], Perdew and Zunger [42] and Yuan and Zhang [43]) as follows

$$\begin{aligned} V_{CP}(r) &= V_{SR}^{Corr}(r), \quad r \le r_0 \\ &= -\frac{\alpha_d}{2r^4}, \qquad r > r_0 \end{aligned} \tag{10}$$

where α_d is dipole polarizability of the target and we have used short range correlation potential similar to [41].

We have also included PCI in our DWBA calculations using the Ward-Macek factor (M_{ee}) [44]. The M_{ee} is defined as

$$M_{ee} = N_{ee}\left|{}_1F_1(-i\nu_3, 1, -2k_3 r_{3ave})\right|^2$$

Where $\nu_3 = -\frac{1}{|k_1 - k_2|}$, $r_{3ave} = \frac{\pi^2}{16\varepsilon}\left(1 + \frac{0.627}{\varepsilon}\sqrt{\varepsilon}\ln\varepsilon\right)^2$, $N_{ee} = \frac{\gamma}{e^{\gamma} - 1}$ here $\gamma = \frac{2\pi}{|k_1 - k_2|}$

ε is the total energy of the two exiting electrons.

The TDCS incorporating PCI through M_{ee} is now written as

$$\frac{d^3\sigma}{d\Omega_1\, d\Omega_2\, dE_1} = M_{ee}(2\pi)^4 \frac{k_1 k_2}{k_0} \sum_{av}\left(|f|^2 + |g|^2 - \mathrm{Re}\left(f^* g\right)\right) \tag{11}$$

3. Results and discussion

The results of triple differential cross sections (TDCS) for the electron impact ionization of Mg (3s) atoms are presented in Figures 1 and 2. The theoretical and experimental results have been normalized to unity at symmetric scattering angle $\theta_1 = 45^0$. The solid curve represents our modified DWBA calculations which include correlation-polarization potential and post collision interaction (DWBACPE calculations), the dashed curve represents our standard DWBA calculations. The solid circles are experimental data of Murray [28]. Till date there are few attempts, as mentioned in the introduction section of this paper, to explain the features of TDCS of doubly symmetric (e, 2e) processes [22, 34] and unequal energy sharing condition [35, 36] on Mg (3s) target. All of these calculations have been done in DWBA formalism and have mix degree of agreement with the experimental results. Hitawala et al. [22] have calculated TDCS using spin averaged static exchange potential [36] and included target polarization in the standard DWBA formalism. Khajuria et al. [34] have reported the results of TDCS using modified semi classical exchange potential [45] and also included PCI using Gamow factor in the standard DWBA formalism.

We present the TDCS results of our DWBA and DWBACPE calculations for the ionization of Mg atom at incident electron energies 17.65, 22.65, 27.65, 37.65, 47.65, 57.65 and 67.65 eV which are 5.0 eV to 30.0 eV above ionization threshold. A two peak structure is observed in the TDCS profile for Mg atom in our calculations as well as in the experimental measurement. The two peak structure is observed up to incident electron energy 37.65 eV and at the other incident electron energies a shallow peak is observed near scattering angle $\theta_1 = 80^0$. This feature of TDCS is visible in our DWBA calculations as well in the experimental results. We observe that the DWBA results including correlation-polarization potential and PCI are able to produce correct position of the forward peak at incident electron energies 17.65, 22.65 and 27.65 eV, which is similar to the direction of forward peak in the experimental results (see solid curve in Fig. 1). We also observe that the DWBACPE calculations are also able to produce the correct position of the dip at the above mentioned incident electron energies, however still there are some discrepancies in the magnitude and direction of backward scattering peak at the incident electron energies 17.65, 22.65 and 27.65 eV. Thus we can state that the polarization and post collisional interaction effects are important at the low energies in the coplanar symmetric geometry and inclusion of these effects in standard DWBA formalism improves the agreement of theoretical results with the experimental data. The DWBA as well as the DWBACPE calculations are in very good agreement with the experimental results in the forward peak region at the other incident electron energies (see Fig. 2). However there are some discrepancies in our theoretical results and experimental data in the backward peak direction. The overall agreement of our present DWBA calculations including correlation-polarization potential and PCI and experimental data is very good.

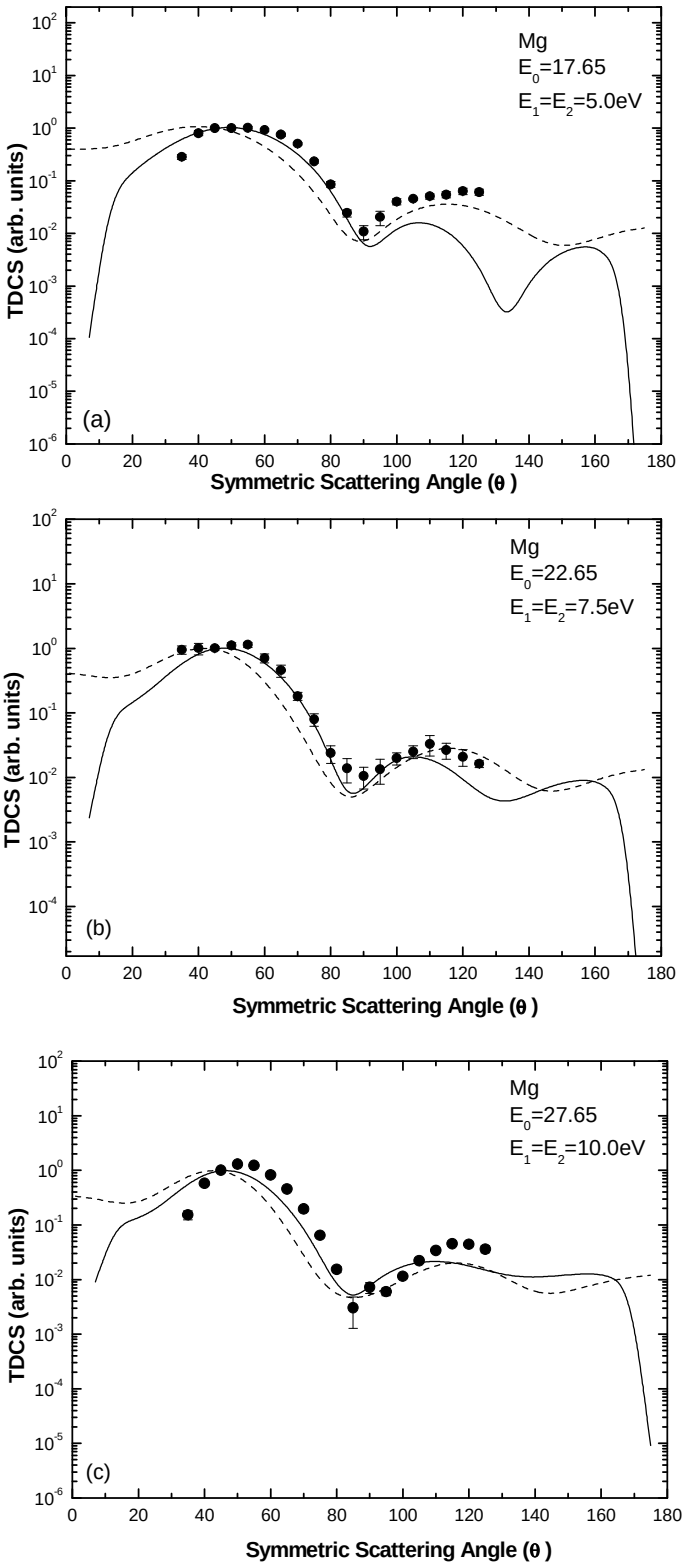


Figure 1: Triple differential cross section of Mg atom as a function of symmetric angle $\theta_1 = -\theta_2 = \theta$ in the coplanar symmetric geometry; symbol (•): experimental data of Murray [28]; Dashed curve: present standard DWBA calculation; Solid curve: present DWBA calculation including correlation-polarization potential and PCI. The experimental and theoretical results have been normalized to unity at symmetric scattering angle $\theta_1 = 45^0$.

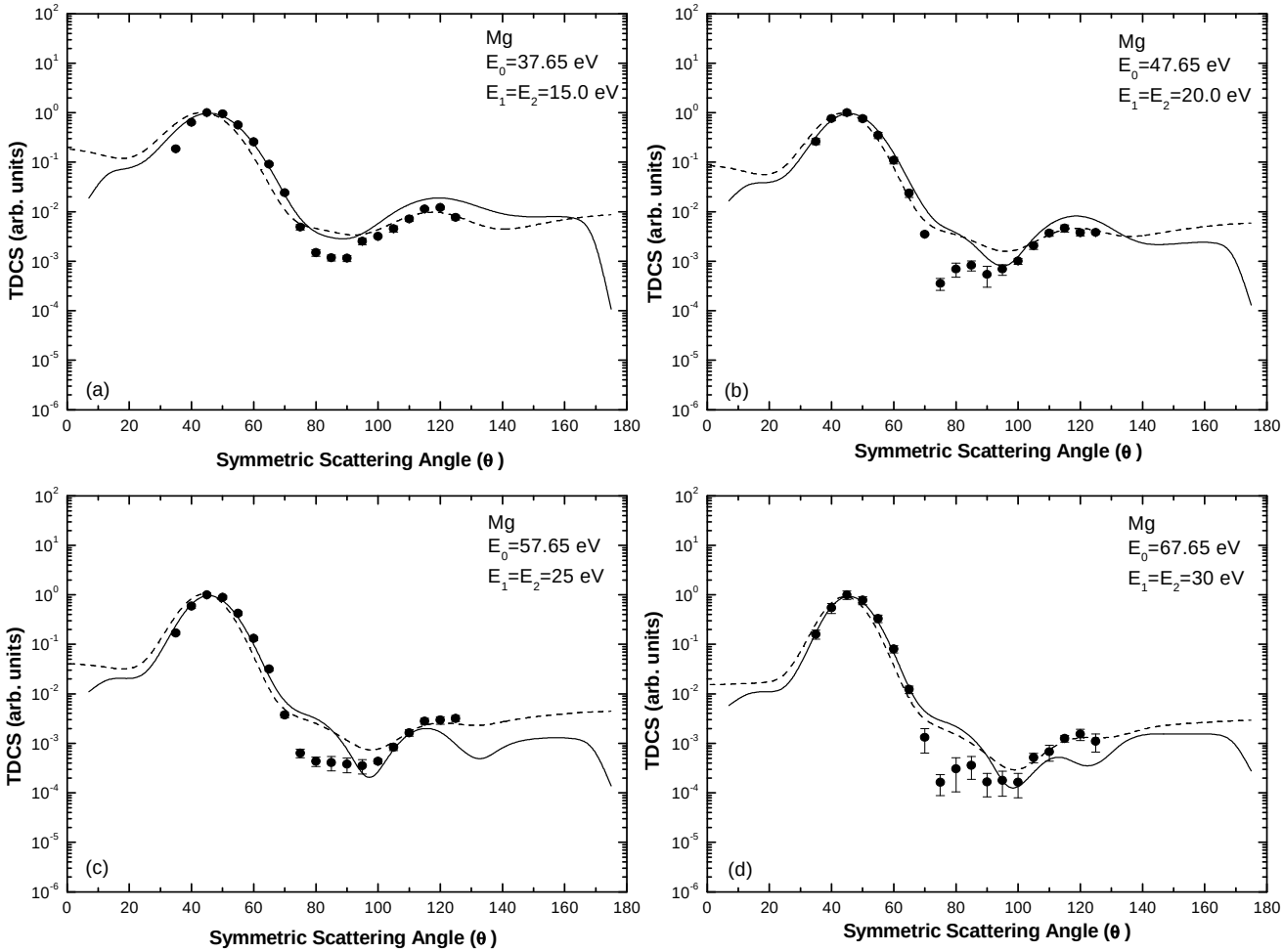


Figure 2: Triple differential cross section of Mg atom as a function of symmetric angle $\theta_1 = -\theta_2 = \theta$ in the coplanar symmetric geometry; symbol (•): experimental data of Murray [28]; Dashed curve: present standard DWBA calculation; Solid curve: present DWBA calculation including correlation-polarization potential and PCI. The experimental and theoretical results have been normalized to unity at symmetric scattering angle $\theta_1 = 45^0$.

We have presented our results for seven incident electron energies (from excess energy 5 eV to 30 eV) on which the measurements are available. We observe that our modified DWBA results (which include correlation-polarization potential and PCI) are able to produce most of the trends of TDCS as observed in the experimental data but still there exist few discrepancies at very low incident electron energies. The polarization effect plays an important role at the incident electron energies used in the present investigation in the coplanar symmetric geometry; however the effect of PCI is only significant for few lower incident electron energies. All the previously available calculations [22, 34] have reasonable amount of agreement with the experimental data but the present attempt further improves the agreement between theory and measurements. Finally, we conclude that further studies with the proper treatment of polarization, exchange, electron correlation and higher order effects are

required to improve the understanding of collision dynamics of alkali atom magnesium in the coplanar symmetric geometry.

Acknowledgements

One of us (VP) acknowledges to the Science and Engineering Research Council (SERC), Department of Science Technology (DST), Govt. of India for the Fast Track Young Scientist Research Grant (SR/FTP/PS-17/2009). We are thankful to Professor Andrew James Murray for providing the experimental data.

References

[1] Ehrhardt H, Schulz M, Tekaat T and Willmann K 1969 Phys. Rev. Lett. **22**, 89.
[2] Rescigno T N, Baertschy M, Isaacs W A and McCurdy C W 1999 Science **286,** 2474.
[3] Bray I, Fursa D V, Kheifets A S and Stelbovics A T 2002 J. Phys. B **35**, R117.
[4] Whelan C T, Allan R J, Walters H R J and Zhang X 1993 (e, 2e) and related processes ed. C. T. Whelan et al. (Dordrechat: Kluwer) p1.
[5] McCarthy I E and Weigold E 1976 Phys. Rep. **C27**, 275.
[6] Byron Jr F W and Joachain C J 1989 Phys. Rep. **179**, 211.
[7] Nakel W and Whelan C T 1999 Phys. Rep. **315**, 409.
[8] Lahmam-Bennani A 1991 J Phys B **24,** 3645.
[9] Whelan C T, Allan R J, Walters H R J and Zhang X 1993 (e, 2e) and related processes ed. C. T. Whelan et al. (Dordrechat: Kluwer).
[10] Whelan C T, Allan R J, Rasch J, Walters H R J, Zhang X, Roder J, Jung K and Ehrhardt H 1994 Phys. Rev. A **50**, 4394.
[11] Bray I, Fursa D V, Roder J and Ehrhardt H 1998 Phys. Rev. A **57**, R3161.
[12] Stelbovics A T, Bray I, Fursa D V and Bartschat K 2005 Phys. Rev. A **71**, 052716.
[13] Bray I 2002 Phys. Rev. Lett. **89**, 273201.
[14] Rioual S, Roder J, Rouvellou B, Ehrhardt H, Pochat A, Bray I and Fursa D V 1998 J. Phys. B **31**, 3117.
[15] Bray I 2000 J. Phys. B **33**, 581.
[16] Pindzola M S et al. 2007 J. Phys. B **40**, R39.
[17] Colgan J, Pindzola M S, Childers G and Khakoo M 2006 Phys. Rev. A **73**, 042710.
[18] Colgan J, Foster M, Pindzola M S, Bray I, Stelbovics A T and Fursa D V 2009 J. Phys. B **42**, 145002.
[19] Biava D A, Saha H P, Engel E, Dreizler R M, McEachran R P, Haynes M A, Lohmann B, Whelan C T and Madison D H 2002 J. Phys. B **35**, 293.
[20] Prideaux A and Madison D H 2003 Phys. Rev. A **67**, 052710.
[21] Prideaux A, Madison D H and Bartschat K 2005 Phys. Rev. A **72**, 032702.
[22] Hitawala U, Purohit G and Sud K K 2008 J. Phys. B **41**, 035205.
[23] Purohit G, Bhullar A S and Sud K K 2003 Indian J. Phys. B **77(2),** 177.
[24] Allan R J, Whelan C T and Walters H R J 1993 J. Phys. IV **3**, 39.
[25] Rioual S, Pochat A, Gelebart F, Allan R J, Whelan C T and Walters H R J 1995 J. Phys. B **28**, 5317.
[26] Whelan C T, Allan R J, Rasch J, Walters H R J, Zhang X, Roder J, Jung K and Ehrhardt H 1994 Phys. Rev. A **50**, 4394.
[27] Murray A J and Cvejanovic D 2003 J. Phys. B **36**, 4875.
[28] Murray A J 2005 Phys. Rev. A **72**, 062711.
[29] Purohit G, Patidar Vinod and Sud K K 2009 Physica Scripta **80,** 065301.
[30] Purohit G, Patidar Vinod and Sud K K 2010 Physics Letters A **374,** 2654.
[31] Bray I, Fursa D V and Stelbovics A T 2008 J. Phys. B **41**, 215203.
[32] Khajuria Y and Deshmukh P C 2008 Phys. Rev. A **78**, 024702.

[33] Chauhan R K, Srivastava M K and Srivastava R 2005 Phys. Rev. A **71**, 032708.
[34] Khajuria Y, Sunil Kumar S and Deshmukh P C 2007 Phys. Rev. A **75**, 022708.
[35] Bolognesi P et al. 2008 J. Phys. B 41, 015201.
[36] Bolognesi P et al. 2008 J. Phys. B 41, 065203.
[37] Clementi E and Roetti C 1974 At. Dat. Nucl. Dat. Tab. **14**, 187.
[38] Furness J B and McCarthy I E 1973 J. Phys. B **6**, 2280.
[39] Riley M E and Truhlar D G 1975 J. Chem. Phys. **63**, 2182.
[40] McCarthy I E 1995 Aust. J. Phys. **48** 1.
[41] Padial N T and Norcross D W 1984 Phys. Rev. A **29**, 1742.
[42] Perdew J P and Zunger A 1981 Phys. Rev. B **23**, 5048.
[43] Yuan J and Zhang Z 1989 J. Phys. B **22**, 2751.
[44] Ward S J and Macek J H 1994 Phys. Rev. A **49**, 1049.
[45] Gianturco F A and Scialla S 1987 J. Phys. B **20**, 3171.