Optical potential approach for positron scattering by metastable 2^3S state of helium*

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The momentum space coupled channels optical (CCO) method for positron scattering has been extended to study the scattering of positrons by metastable helium for impact energies in the range from the positronium threshold up to high energies. Both the positronium formation and ionization continuum channels are included in the calculations via a complex equivalent local potential. The positronium formation, ionization, elastic and 2^3S–2^3P excitation, and total scattering cross sections are all presented and compared with the available information.

Keywords: positron, excited, helium, positronium formation

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1. Introduction

Although the studies of interactions of slow positrons with ground state atoms have been the subject of intense interest in atomic physics for more than two decades, the interactions of slow positrons with excited atoms has been only exiguously investigated.[1,2] Investigations of interactions of slow electrons with excited atoms also are relatively recent, but large differences are revealed in the dynamics of a collision for electron scattering from excited atoms as compared with corresponding ground state atoms.[3,4] Excited atoms are known to have large polarizabilities, low excitation and ionization thresholds that can dramatically affect the behavior of the dynamics of a collision.

In view of these differences between electron scattering by ground state and excited state atoms, we realized that the dynamics of positron collision with excited atoms are expected to be significantly different from the analogous collisions involving ground state atoms, since the positron-atom problem is more complex than the electron case. In spite of the absence of exchange interaction, we still expect that the studies of the interaction of positrons with excited atoms can provide new insight into the details of positron-atom interactions due to the added richness of positronium channels.

We employ metastable helium as a test ground of the study of slow positron scattering by excited atoms, of special interest is the positronium formation (Ps-formation) rearrangement channel which is open at all impact energies for this system. The interactions of slow positrons with many-electron atoms are characterized by strong correlation effects that may be exemplified through the process of Ps-formation. Including these channels is critical to understand collisions of positron-excited atom systems. Despite there being significant progress in theoretical descriptions of the charge transfer rearrangement process during the past decades and a number of approaches have been employed to study the Ps-formation channel for positron collisions with ground state atoms,[5–14] Ps-formation for positron scattering on excited atoms remains a challenge and the underlying physics of this process has yet to be elucidated.[1] The only available reports on the work of Ps-formation in positron-excited atom systems are the convergent close-coupling calculation (CCC) from Utamuratov *et al.*[15] and the work of Hanssen *et al.*,[15] in which they studied Ps-formation in excited helium using a four-body version of the continuum distorted wave approach at intermediate and high positron impact energies, which is not involved in the present work.

In addition to the charge transfer process, there is a very important process of ionization that is sensitive to the correlation dynamics of three-body interaction,[4,16] and the low ionization threshold of the excited atoms makes ionization energetically a more favorable process. Thus it is very important to incorporate the continuum channel to correct the treatment of positron scattering problems.

In the present work, the coupled channel optical potential (CCO) method of positron–atom collision[5] has been extended to study the interactions of a positron with a metastable helium 2^3S state, in which all reaction channels can be taken into account via an equivalent local potential that is an *ab initio* complex correlation-polarization potential.[17] The real part of the potential represents the virtual Ps-formation and dynamic

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polarization of the target. At large distances, it has asymptotic behavior: $\alpha/2r^4$, where α is the dipole polarizability of the atom. The imaginary part of the potential describes the rearrangement channels i.e., Ps-formation and continuum states of the target. The validity of the potential has been verified by generating satisfactory scattering cross sections for all reaction channels, especially for the Ps-formation channel at near threshold and lower impact energies for positron scattering on ground-state helium.[18] It is the first time that the method has been applied to study a positron-excited helium system. The contributions of the charge transfer and ionization continuum channels have been estimated by calculating their cross sections for a positron–metastable helium system.

2. Detailed of the calculation method

The total cross section for excitation of the target is calculated by solving the coupled-channel optical equations[5]

$$\langle \boldsymbol{k}i|T|0\,\boldsymbol{k}_0\rangle = \langle \boldsymbol{k}i|V^{(Q)}|0\,\boldsymbol{k}_0\rangle + \sum_{j\in P}\int \mathrm{d}^3k'\langle \boldsymbol{k}i|V^{(Q)}|j\boldsymbol{k}'\rangle \frac{1}{E^{(+)}-\varepsilon_j-1/2k'^2}\langle \boldsymbol{k}'j|T|0\,\boldsymbol{k}_0\rangle, \quad i\in P. \tag{1}$$

Here the space of the target states has been split into P and Q parts. The P space consists of some discrete channels, for example in the present work they are the channels with target excitations from the 2^3S states to the 2^3S, 2^3P, 3^3S, 3^3P, 3^3D, 4^3S, 4^3P, 4^3D states. The Q space includes target ionization continuum and positronium pickup channels via an *ab initio* optical potential $V^{(Q)}$ that is a complex polarization potential $W^{(Q)}$ added to the channel-coupling potentials.

$$W^{(Q)} = W_{\mathrm{I}}^{(Q)} + W_{\mathrm{Ps}}^{(Q)}, \tag{2}$$

where $W_{\mathrm{I}}^{(Q)}$ and $W_{\mathrm{Ps}}^{(Q)}$ stand for the parts of the polarization potential that describe the ionization continuum and the positronium formation rearrangement process, respectively. The form used here for the matrix element of the polarization potential is given by

$$\langle \boldsymbol{k}', \mathrm{i}|W^{(Q)}|j,\boldsymbol{k}\rangle = \sum_{n\in Q}\langle \boldsymbol{k}'i|V|\Psi_n^{(-)}\rangle \frac{1}{E^{(+)}-E_n}\langle \Psi_n^{(-)}|V|j\boldsymbol{k}\rangle, \tag{3}$$

here $\Psi_n^{(-)}$ represents the time reverse of the exact state vector for a reaction starting in channel n. Spin dependence is implicit in the notation.

For the breakup process, the model used is

$$|\Psi_n^{(-)}\rangle = |c\psi^{(-)}(\boldsymbol{q}_<)\boldsymbol{q}_>\rangle, \tag{4}$$

where $\boldsymbol{q}_<$ and $\boldsymbol{q}_>$ are the greater and lesser of the absolute momenta of the outgoing particles, respectively. Ionization is described in a quasi three-body model, where c is the remaining core He^+ in its ground state 1s. $\langle \boldsymbol{r}|\psi^{(-)}(\boldsymbol{q}_<)\rangle$ is a Coulomb wave orthogonalized to the orbital 2s, from which the electron is removed. If the slow particle is a positron the appropriate Coulomb wave is used. $\langle \boldsymbol{r}|\boldsymbol{q}_>\rangle$ represents a plane wave.[19,20]

The approximation model used for positronium formation is

$$|\Psi_n^{(-)}\rangle = (1-|\psi_i\rangle\langle\psi_i|)|\sum_{\mu}|c\phi_\mu \boldsymbol{k}_{\mathrm{ps}}\rangle, \tag{5}$$

where $\phi_\mu^{(-)}$ is the bound state of the positronium and $\boldsymbol{k}_{\mathrm{ps}}$ is the momentum of the positronium center of mass that is presented by a plane wave $\langle \boldsymbol{R}|\boldsymbol{k}_{\mathrm{ps}}\rangle$, since only short-range terms in the positronium–ion potential survive. $\boldsymbol{R}$ is the coordinate of the positronium center of mass.

$$\boldsymbol{R} = \boldsymbol{r}_{\mathrm{p}} + \boldsymbol{r}_{\mathrm{e}}, \tag{6}$$

where $\boldsymbol{r}_{\mathrm{p}}$ and $\boldsymbol{r}_{\mathrm{e}}$ are the coordinates of the positron and the electron respectively. Here ψ_i is the target states, and the wave function is orthogonalized to the metastable state of 2s, from which the electron is captured. We use this approximation to describe hole–particle interactions and Coulomb screening, the important many-body effects.

The notation n is a discrete notation for the two-body rearrangement channels. The optical potential matrix element for positronium formation is

$$\langle \boldsymbol{k}'i|W_{\mathrm{Ps}}^{(Q)}|j\boldsymbol{k}\rangle = \sum_n \langle \boldsymbol{k}'i|V|\Psi_n^{(-)}\rangle \frac{1}{E^{(+)}-E_n}\langle \Psi_n^{(-)}|V|j\boldsymbol{k}\rangle, \tag{7}$$

here

$$(\varepsilon_j - H_T)|j\rangle = 0. \tag{8}$$

The independent-particle model has been used for calculating the positronium formation matrix element. The metastable state 2s of helium is represented by a Hatree–Fock wave function and expanded by STO's bases.

The amplitude of the positronium formation potential has been calculated by using the numerical method of Cheshire.[21] In the present calculation, the P space consists of eight channels: $2,3,4^3S$; $2,3,4^3P$; $3,4^3D$. The optical potential describing the three-body ionization and two-body rearrangement channels are in the channel-couplings. The target bound states are represented by configuration (CI) wave functions. The basis used in the CI representation of these states consists of nine orbitals represented by the STO's basis, namely, $1,2,3,4$s; $2,3,4$p; $3,4$d, orbitals and the pseudo-orbitals, $\bar{\mathrm{s}}$, $\bar{\mathrm{p}}$, and $\bar{\mathrm{d}}$.

Finally, the total ionization cross section is estimated by

$$\sigma_{\rm I} = (2/k)(2\pi)^3 {\rm Im}\langle \boldsymbol{k}\,0|W_{\rm I}^{(Q)}|0\,\boldsymbol{k}\rangle, \quad (9)$$

and the total positronium formation cross section is

$$\sigma_{\rm ps} = (2/k)(2\pi)^3 {\rm Im}\langle \boldsymbol{k}\,0|W_{\rm Ps}^{(Q)}|0\,\boldsymbol{k}\rangle. \quad (10)$$

3. Results and discussion

The present total Ps-formation cross sections (in $n = 1$ and $n = 2$ states) for positron impact on helium from the metastable 2^3S state are compared with the CCC calculation results[2] in Fig. 1 and exhibit significantly different behavior especially at very low energies. The present Ps-formation cross section shows a monotonously decreasing behavior from its maximum at zero incident energy as incident energy increases, while the CCC cross sections have a peak position around 2 eV. The difference is mainly due to the different treatment of the positronium formation process and the different description of the correlation effect that is enhanced in the case of positron scattering with an excited atom. An *ab initio* complex correlation-polarization potential[17] is adopted in our calculation to incorporate the positronium formation channels while the pseudo-states expansion is used in the CCC calculation. Both methods have been validated in the prediction of various cross sections for positron scattering with helium from its ground state. The exact origin of the discrepancies between both calculations and more accurate details at low energy positron impact on helium from excited states need to be revealed by more theoretical and experimental work.

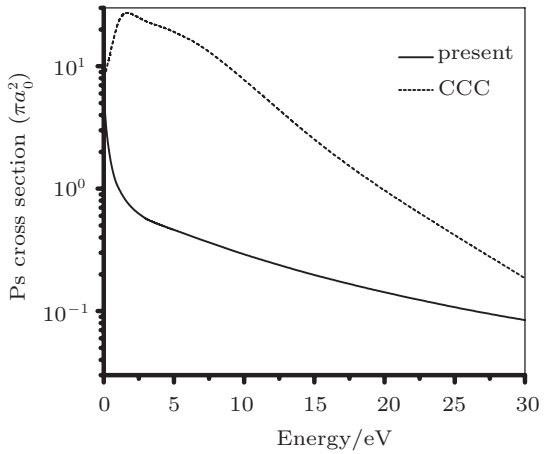


Fig. 1. Total Ps-formation cross sections of positron impact on helium from metastable state (2^3S) compared with the CCC results.[2] Solid line: present results; dashed line: CCC results.

In Fig. 2, the comparisons between the present Ps formation cross sections for positron-metastable state helium and our previous Ps cross sections for positron-ground state helium[18] are shown as functions of the incident positron energies. There is an evident difference in the energy dependance of the Ps-formation cross section between positron collisions with ground-state and excited state helium. Comparing with the monotonously decreasing behavior for the metastable helium case, the Ps-formation for positron-ground state helium gradually rises to its peak value firstly then descends as impact energies increase. Another remarkable feature of the excited state case is its large values that are up to 4 times the Ps cross sections in the positron-ground state of the helium system. The differences are due to the low binding energy of 2^3S of helium that is less than the bound energy of Ps-formation 6.8 eV. The smaller ionization potential makes the values of the Ps-formation cross section very large,[17] since this process is less virtual.

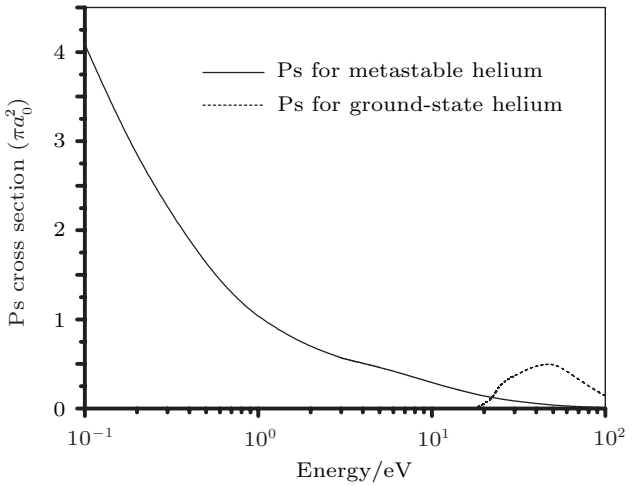


Fig. 2. Total Ps-formation cross sections of positron impact on helium from metastable state (2^3S) and ground state. Solid line: metastable state; dashed line: ground state.

In the present calculation, we have not incorporated the appropriate channels supporting bound state $e^+He(^3S)$, since for an atom A with the ionization potential close to 6.8 eV, the positron–atom bound state wave function is not described very well by the e^+A component and the positron–atom complex has rather a molecule-like structure. Its wave function can be qualitatively described as a linear combination of the e^+A and PsA^+ component.[22,23] Rienzi and Drachman have estimated the cross section of the forming system in the process that was very small, the bound state is best described not as a positron bound to the triple state helium atom but as a positronium atom bound loosely to a helium ion.[24] In order to check correlation effects, we have also calculated the Ps-formation potential with and without electron–hole interaction and the screening effects in both cases of positron impact on metastable state helium and ground state helium. The calculations indicated that the effects of electron–hole interactions and screening in atoms in the positron-ground state helium case are more than 10 times larger than in the positron-excited helium case at near Ps threshold and are decreasing as impact energies are increasing. Comparing the ratios of amplitudes of Ps-formation cross sections in $n = 2$ to $n = 1$ states

for positron impact on metastable state and ground state helium, we found that positron-helium in the ground state has a larger ratio, and this indicates that polarization of Ps atom by ionic field for positron-excited atom systems is much less than positron-ground atom systems. Thus the plane wave approximation for positronium formation should be satisfied.

In Fig. 3, we present the cross sections for elastic scattering and electronic excitation from the 2^3S to the 2^3P state by positron impact comparing with the CCC results.[2] Those two calculations show a similar tendency for both elastic and excitation cross sections while a similar discrepancy compared with the case of positronium formation cross sections that occur at the very low energies in the elastic cross section. This is also possibly due to the different treatment of the correlation effect. By comparing the elastic and excitation cross sections with the total cross sections, one can find that the cross sections of electron excitation from the 2^3S to the 2^3P state, the lowest resonance transition at low impact energies, exceeds the cross sections for elastic scattering and dominates the total cross sections at energies above 4 eV. The behavior of the cross sections indicates that the long-range dipole polarization potential plays a significant role and dominates the whole scattering process. This is very similar to the case of electron scattering by excited helium.[25]

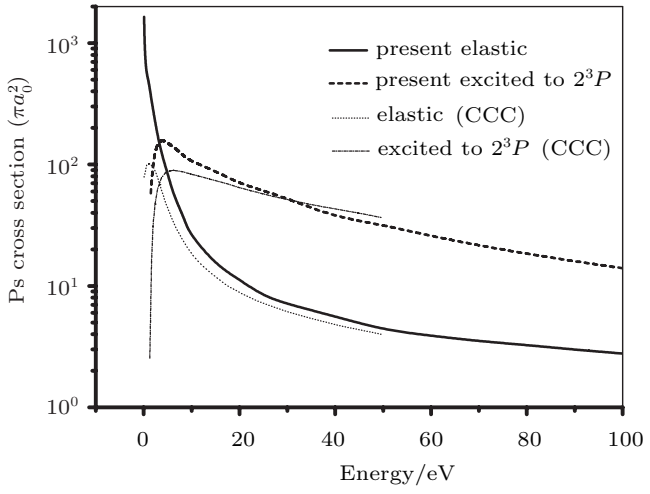


Fig. 3. The present and CCC[2] elastic scattering and 2^3S–2^3P excitation cross sections. Solid line: present elastic scattering; dashed line: present 2^3S–2^3P excitation; dotted line: elastic scattering (CCC); dashed–dotted line: 2^3S–2^3P excitation (CCC).

The present and CCC ionization cross sections for positron scattering from the lowest triple state of helium as well as with the present results for the case of ground-state helium are presented in Fig. 4. Compared with the CCC results, the present cross section for the case of an excited state has a similar peak position around 15 eV but is significantly lower between 8 eV and 50 eV. The present ionization cross sections are calculated using the optical theorem and a complex optical potential describing the ionization channel while the CCC calculation uses a large number of pseudo states to represent the continuum states. The comparison between the two CCO ionization cross sections demonstrated very significant differences between the behavior of ionization for positron impact helium from the excited state and ground state at low and intermediate incident energies. The lower ionization threshold energy and the higher polarization of the excited states of helium compared to the ground state case cause a shift of the ionization cross section to lower energies and an enhancement in its magnitude. At high impact energies above 400 eV, the ionization cross sections for the excited state decrease more quickly than the ground state case.

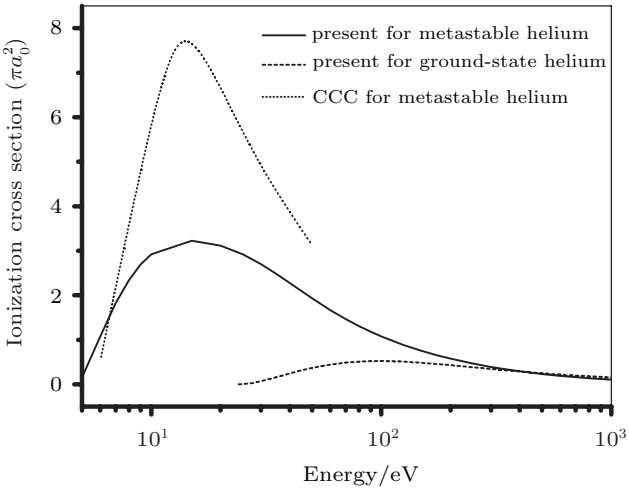


Fig. 4. Present ionization cross sections of positron scattering from the metastable state (2^3S) and ground state of helium compared with the CCC results for metastable state (2^3S). Solid line: metastable state; dashed line: ground state; dotted line: CCC results.

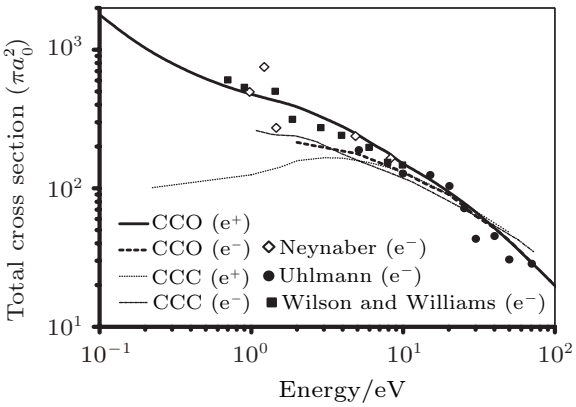


Fig. 5. Total cross sections for positron and electron scattering from metastable helium (2^3S). Solid line: present results for positron; dashed line: previous CCO results for electron; dotted line: positron CCC; dotted line: electron CCC; diamond: Neynaber *et al.*;[26] blacksquare: Wilson and Williams;[25] bullet: Uhlmann *et al.*[4]

The present total scattering cross sections, which is the sum of cross sections of positronium formation, ionization, elastic scattering, and the excitation from the initial state to all other discrete states in P space, for positron and electron impact on the helium from the 2^3S state are displayed in Fig. 5, and the experimental measurement results of Neynaber *et al.*,[26] Uhlmann *et al.*,[4] and Wilson and Williams[25]

for electron scattering, the theoretical results of the CCC calculation[2,27] for both positron and electron scattering, and the previous CCO calculation for the electron case[28] are also shown. The present result is illustrated by the solid curve that is close to electron total cross sections of the existing experimental measurements and theoretical calculations in both shape and magnitude at energies above 20 eV, and both the positron and electron cross sections tend to merge at high impact energies. The comparison with total electron scattering cross sections indicates that the exchange effect between the incident and the bound electrons generally does not influence significantly the overall behavior of excited atom scattering. At lower energies, the total cross section for the positron case are significantly larger than for the electron case. The difference may be attributed to the contribution from Ps-formation, the rearrangement channel.

The present total scattering cross sections are presented in Fig. 6 and compared with the CCO total cross section for positron impact on ground state helium[18] and CCC cross sections for metastable helium. Once again the present cross sections and the CCC calculations are very close to each other at energies above 10 eV while they have different behavior at very low energies. The origin of the discrepancy needs more theoretical and experiment work to resolve. The comparison between the present total cross sections for the excited state case and ground state case shows that the cross section for the excited state exceeds the total cross section for the ground state by about two orders of magnitude. This large enhancement in the total cross section is attributed to the much higher value of the dipole polarizabitity of He (2^3S) compared to He ($^1S_0$).

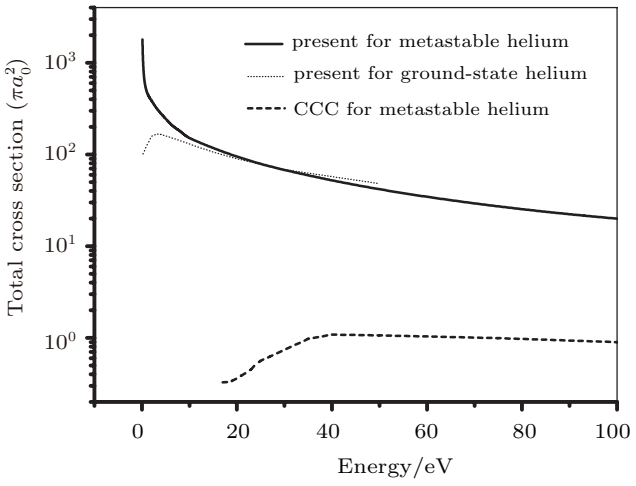


Fig. 6. Total scattering cross sections of positron impact on helium from its metastable state (2^3S) and ground state along with the CCC results for metastable state (2^3S). Solid line: metastable state; dashed line: ground state; dotted line: CCC.

4. Conclusion

In the present work, the positronium formation, ionization, elastic and 2^3S–2^3P excitation, and total scattering cross sections have been calculated for positron impact on the metastable 2^3S state of helium. Investigations have been performed by the positron coupled channels optical method in which an equivalent and local potential is developed to treat the Ps-formation and ionization continuum. For these studies, we find significant differences between the dynamics of positron collisions with excited and ground state helium at low impact energies. Interactions of slow positrons with excited helium are characterized by extremely large cross sections. Comparing with the recent CCC calculations,[2] our results for metastable helium agree well at higher energies but exhibit different features at the very low energy region. Experimental measurements that as yet have not been done are expected to reveal more details of positron impact on the metastable 2^3S state of helium.

References

[1] Surko C M, Gribakin G F and Buckman S J 2005 *J. Phys. B: At. Mol. Opt. Phys.* **38** R57

[2] Utamuratov R, Kadyrov A S, Fursa D V, Bray I and Stelbovics A T 2010 *Phys. Rev. A* **82** 042705

[3] Christophorou L G and Olthoff J K 2001 *Adv. At. Mol. Opt. Phys.* **44** 155

[4] Uhlmann L J, Dall R G, Truscoff A G, Hoogerland M D, Beldwin K G H and Buckman S J 2005 *Phys. Rev. Lett.* **94** 173201

[5] Zhou Y, Ratnavelu K and McCarthy I E 2005 *Phys. Rev. A* **71** 042703

[6] Nan G, Zhou Y and Ke Y 2004 *Chin. Phys. Lett.* **21** 2406

[7] Kothari H N and Joshipura K N 2010 *Chin. Phys. B* **19** 103402

[8] Mandal P, Guha S and Sil N C 1979 *J. Phys. B: At. Mol. Phys.* **12** 2913

[9] Igarashi A and Toshima N 1992 *Phys. Lett. A* **164** 70

[10] Schultz D R and Olson R E 1988 *Phys. Rev. A* **38** 1866

[11] Champell C P, McAlinden M T, Kernoghan A A and Walters H R J 1998 *Nucl. Instrum. Phys. Res. B* **143** 41

[12] Hewitt R N, Noble C P and Bransden B H 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** 557

[13] Mitroy J 1996 *J. Phys. B: At. Mol. Opt. Phys.* **29** L263

[14] Kodysov A S and Bray Igor 2002 *Phys. Rev. A* **66** 012710

[15] Hanssen J, Hervieux P A, Fojon F A and Rivarola R D 2000 *Phys. Rev. A* **63** 012705

[16] Bartschat K 2002 *J. Phys. B: At. Mol. Opt. Phys.* **35** L527

[17] Gribakin F and Ludlow J 2004 *Phys. Rev. A* **70** 032720

[18] Cheng Y and Zhou Y 2007 *Phys. Rev. A* **76** 012704

[19] McCarthy I E and Stelbovics A T 1980 *Phys. Rev. A* **22** 502

[20] McCarthy I E and Zhou Y 1994 *Phys. Rev. A* **49** 4597

[21] Cheshire I M 1964 *Proc. Phys. Soc.* **83** 227

[22] Mitroy J, Bromley M W J and Ryzhikh G G 2002 *J. Phys. B: At. Mol. Opt. Phys.* **35** R81

[23] Dzuba Y A, Flanbaum V V, Gribakin G F and King W A 1996 *J. Phys. B: At. Mol. Opt. Phys.* **29** 3151

[24] Rienzi J D and Drachman R J 2006 *Phys. Rev. A* **73** 012703

[25] Wilson W G and Williams W L 1976 *J. Phys. B: At. Mol. Phys.* **9** 423

[26] Neynaber R H, Trujillo S M, Marino L Land Rothe E W 1964 *Atomic Collision Processes: Proceedings of the Third International Conference on the Physics of Electronic and Atomic Collisions*, July 22–26, 1963

[27] Fursa D and Bray I 1997 *J. Phys. B: At. Mol. Opt. Phys.* **30** 757

[28] Wang Y C, Zhou Y, Cheng Y, Ratnavelu K and Ma J 2010 *J. Phys. B: At. Mol. Opt. Phys.* **43** 045201