# Electron-impact excitation of zinc and ytterbium atoms

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Relativistic distorted wave calculations have been carried out to study the electron-impact excitation of Zn and Yb atoms from their ground $^1S_0$ state which have outer shell configurations $3d^{10}4s^2$ and $4f^{14}6s^2$, respectively. Excitations to the lowest and next-lowest singlet $P$ states *viz*. $(4s4p, 4s5p)\ ^1P_1$ in Zn and $(6s6p, 6s7p)\ ^1P_1$ in Yb along with the $(6s5d)\ ^1D_2$ state in Yb have been considered. Differential and integrated cross section results have been obtained and compared with recent experimental results and theoretical convergent close coupling calculations. In general, good agreement between the theoretical calculations and experimental measurements has been observed.

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## I. INTRODUCTION

There has been renewed interest in studying electron-impact excitation from the ground state of zinc and ytterbium atoms over the last few years [1–8] due to the importance of such processes in plasma studies. For example, there is the possibility of using zinc as a replacement for mercury in high-pressure discharge lamps [9]. As well, ytterbium has been of interest in biophysical research, where it has been used in the dry film method for the determination of glucose in blood plasma [10]. In addition to the requirement for accurate collision cross section data both of these atoms show strong relativistic spin-orbit and exchange effect contributions which reveal the break down of LS coupling [5,11–13]. There have been limited theoretical investigations of electron scattering from zinc and ytterbium in the past and a systematic treatment of such processes is very desirable.

In the earliest study of inelastic scattering from zinc, Williams and Bozinis [14] measured differential cross sections (DCSs) for the excitation of the $(4s4p)\ 4\ ^1P_1$ and $(4s5p)\ 5\ ^1P_1$ states from the ground state but only at a single incident electron energy of 40 eV. Kaur *et al*. [15], in a paper mainly devoted to the excitation of magnesium, also reported fully relativistic distorted wave (RDW) calculations for the electron-impact excitation of the $4\ ^1P_1$ and $4\ ^3P_{0,1,2}$ states of zinc at incident electron energies of 10, 20, and 40 eV to encourage more experimental work on this atom. More recently, Panajotović *et al*. [1] reported DCS measurements for the excitation of the $4\ ^1P_1$ and $5\ ^1P_1$ states of zinc for scattering angles up to $12^\circ$ at low to intermediate electron energies. These DCS measurements were later extended to scattering angles up to $150^\circ$ and were presented along with nonrelativistic convergent close coupling (CCC) calculations in the paper of Fursa *et al*. [2]. In this paper they also compared their theoretical and experimental DCS results with the previous calculations of Kaur *et al*. [15] for the excitation of the $4\ ^1P_1$ state. Although the RDW calculations of Kaur *et al*. [15] were fully relativistic, they used simple single-configuration bound-state wave functions and the results were not in as good agreement with the experimental measurements as the later CCC calculations [2].

For electron scattering from ytterbium, the first measurements of electron-impact coherence parameters for Yb were reported by Li and Zetner [11] at 20 and 40 eV incident electron energies for near forward scattering angles. They detected the electrons which had been superelastically scattered from the laser-excited $6s6p\ ^3P_1$ state of $^{74}$Yb which is de-excited to its ground $6s^2\ ^1S_0$ state. Prompted by such experiments, Srivastava *et al*. [13] carried out the first completely relativistic distorted-wave calculations for the time reversed process, that is, the electron-impact excitation of the $^3P_1$ fine-structure levels of the $6s6p$ state of this atom. They included excitations of all the fine-structure levels of the $6s6p\ ^3P$ state as well as the $6s6p\ ^1P$ state from the ground $6s^2\ ^1S_0$ state and reported a selection of collision parameters including DCSs as well as various Stokes parameters at 20 and 40 eV. These results were again obtained by using only single-configuration bound-state wave functions. Thereafter a series of experiments at the University of Manitoba were conducted to study electron scattering from ytterbium [5,6,12,16]. Johnson *et al*. [16] have measured the DCS for excitation of the $6s6p\ ^1P_1$ state at impact energies of 5, 10, 20, 40, and 80 eV while Zetner *et al*. [12] studied electron-impact excitation of the $6s6p\ ^3P_{0,1,2}$ levels and reported measurements of DCS and Stokes parameters at collision energies of 10, 20, and 40 eV. In these two experimental papers [12,16] results were reported only up to $50^\circ$ scattering angles. They also reported a comparison with nonrelativistic unitarized distorted wave approximation (UDWA) calculations [17] and the RDW results of Srivastava *et al*. [13]. Reasonably good agreement was found among the two theoretical calculations and the experimental results. More recently the Belgrade group, Predojević *et al*. [3,4], measured DCSs for the excitations of the $(6s6p)\ ^{1,3}P_1$, $(6s5d)\ ^1D_2$, and $(6s7p)\ ^1P_1$ states at a number of incident electron energies in the range 10–80 eV and for a wide range of scattering angles ($1^\circ$–$150^\circ$). They compared their DCS results for the $6s6p\ ^{1,3}P_1$ levels with the UDWA and RDW calculations at 10, 20, and 40 eV but no theoretical results were available at other energies or for the other excited states. Very recently, Bostock *et al*. [8], in light of the new experimental DCS

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results as well as the lack of a comprehensive theoretical study of electron scattering of ytterbium, applied the convergent close-coupling method in both the relativistic (RCCC) and nonrelativistic (CCC) forms to this problem. They reported differential and integrated cross sections for excitation of the $(6s6p)\ ^3P_{0,1,2}$, $(6s6p)\ ^1P_1$, $(6s7p)\ ^1P_1$, and $(6s5d)\ ^1D_2$ states for a wide range of incident electron energies. They found reasonable agreement between their theoretical calculations and the experimental measurements for the various cross sections.

In view of the latest detailed experimental measurements and the nonperturbative CCC and RCCC calculations reported for electron excitation from the ground state of zinc [2] and ytterbium [8] atoms, in the present work we have repeated our earlier RDW calculations using elaborate multiconfiguration wave functions for the bound states and present our improved results for the DCS and integrated cross sections (ICS) for excitation of the singlet states of these two atoms in order to establish the reliability of widely used perturbative approaches at least in the range of intermediate and high incident electron energies. We have already carried our similar calculations for the excitation of the $(6s6p)\ ^3P_1$ of Yb which were reported in Ref. [5]. The recent applications of our improved RDW approach to electron-impact excitation of various atoms, *viz*. Ca [18], Hg [19], and the inert gases [20,21], where we have used elaborate multiconfiguration wave functions to describe the target atoms, have proved to be very successful. These new RDW calculations for the excitation of Zn and Yb replace our earlier work [13,15] using simpler bound-state wave functions in order to test the reliability of the RDW method for these processes in Yb and Zn as well as future applications for other atoms. In this paper we have applied the RDW method to the electron-impact excitations of the $4\ ^1P_1$ and $5\ ^1P_1$ states of zinc and the $6\ ^1P_1$, $7\ ^1P_1$, and $5\ ^1D_2$ states of ytterbium and report detailed differential and integrated cross sections results. We compare these results with the latest experimental measurements and theoretical CCC and RCCC calculations.

The details of our RDW method used in the present work have been given in our various recent papers [18–21]. In Sec. II, we briefly describe the calculations of the multiconfiguration bound-state wave functions of zinc and ytterbium atoms used in our calculation and give the formula for calculating cross sections. We present our results in Sec. III and draw some overall conclusions in Sec. IV.

## II. THEORY

The RDW method is a perturbative method involving only the configurations of the initial and final states of the target. This is in contrast to multichannel methods such as the CCC and RCCC which include a large number of excited states in the expansion of the wave function. The RDW method gives reliable results at medium and high incident electron energies and has the advantage of requiring much less computational power than multichannel methods. Methods such as the CCC are more reliable at lower energies but become more difficult to calculate as the energy increases.

Since we include only first-order terms in our calculations, configurations included in the initial and final wave functions can only differ by one orbital. We include sufficient configurations in our multiconfiguration wave functions to ensure the energy of the states and the oscillator strengths (in the case of allowed dipole excitations) have good accuracy. Generally, we find that wave functions with the smallest number of configurations which meet our accuracy criteria give the most reliable cross sections over a wide range of energies.

The nuclear charges of Zn and Yb are 30 and 70, respectively, and both atoms have two valence electrons in their ground states with configurations $[\mathrm{Ar}]3\bar{d}^4 3d^6 4s^2$ and $[\mathrm{Xe}]4\bar{f}^6 4f^8 6s^2$ using the $j$-$j$ coupling notation as described by Grant [22]. Here $\bar{d}, d, \bar{f}, f$ denote $d$ and $f$ electron orbitals having total angular momentum $j$ of 3/2, 5/2, 5/2, and 7/2, respectively. The transitions considered in the present work are $n\ ^1S_0 \rightarrow n'\ ^1P_1$ for Zn ($n' = 4, 5$) and Yb ($n' = 6, 7$) and also $5\ ^1D_2$ for Yb. These arise due to electron-impact excitation of one valence electron from the ($\mathrm{ns}^2$) ground state configuration to either $n'\bar{p}$ or $n'p$ for the $n'\ ^1P_1$ excitations as well as to either $5\bar{d}$ or $5d$ for the $5\ ^1D_2$ excitation. The ground states for Zn and Yb have even parity and total angular momentum $J = 0$ while the excited $P$ states have odd parity with total angular momentum $J = 1$ and the excited $D$ states have even parity with total angular momentum $J = 2$. To obtain relativistic multiconfiguration wave function for the ground as well as excited states of Zn and Yb we have used the Dirac-Fock GRASP2K program of Jönsson *et al*. [23]. The singlet $P$ excited levels with odd parity and $J = 1$ are connected to the ground states with even parity and $J = 0$ by dipole-allowed transitions. The dipole oscillator strengths for these transitions have also been obtained from GRASP2K code.

The following set of multiconfiguration wave functions for the ground and the first excited states of Zn ($n = 4$) and Yb ($n = 6$) have been obtained as

$$n\ ^1S(J=0) : a_1(ns^2)_{J=0} + a_2(nsn's)_{J=0} + a_3(n\bar{p}^2)_{J=0} + a_4(n\bar{p}n'\bar{p})_{J=0} + a_5(np^2)_{J=0} + a_6(npn'p)_{J=0} + a_7(n's^2)_{J=0} + a_8(n'\bar{p}^2)_{J=0} + a_9(n'p^2)_{J=0} \quad (1)$$

and

$$n\ ^1P(J=1) : b_1(nsn\bar{p})_{J=1} + b_2(nsnp)_{J=1} + b_3(nsn'\bar{p})_{J=1} + b_4(nsn'p)_{J=1} + b_5(n\bar{p}n's)_{J=1} + b_6(npn's)_{J=1} + b_7(n'sn'\bar{p})_{J=1} + b_8(n'sn'p)_{J=1}, \quad (2)$$

where $n' = n + 1$ and the mixing coefficients $a_i$'s and $b_i$'s have been obtained from the GRASP2K code and are given in Table I.

TABLE I. The mixing coefficients $a_i$'s and $b_i$'s in Eqs. (1)–(5) obtained from GRASP2K [23] for the ground- and excited-state wave functions for the various transitions considered in Zn and Yb.

| Mixing coefficients | Zn | Yb | | Mixing coefficients | Zn | Yb | |
|---|---|---|---|---|---|---|---|
| Ground state | $4\,^1S_0 \rightarrow 4\,^1P_1$ | $6\,^1S_0 \rightarrow 6\,^1P_1$ | $6\,^1S_0 \rightarrow 5\,^1D_2$ | Excited state | $4\,^1S_0 \rightarrow 4\,^1P_1$ | $6\,^1S_0 \rightarrow 6\,^1P_1$ | $6\,^1S_0 \rightarrow 5\,^1D_2$ |
| $a_1$ | 0.9700 | 0.9664 | 0.9882 | $b_1$ | 0.4780 | 0.4721 | −0.5684 |
| $a_2$ | −0.0543 | 0.0185 | −0.0448 | $b_2$ | 0.6967 | 0.7352 | 0.7067 |
| $a_3$ | 0.1292 | 0.1648 | −0.0945 | $b_3$ | −0.3094 | −0.2967 | −0.1157 |
| $a_4$ | 0.0512 | 0.0526 | −0.1121 | $b_4$ | −0.4247 | −0.3854 | 0.1049 |
| $a_5$ | 0.1739 | 0.1785 | | $b_5$ | −0.0517 | 0.0016 | −0.1463 |
| $a_6$ | 0.0759 | 0.0612 | | $b_6$ | 0.0738 | −0.0021 | −0.2385 |
| $a_7$ | −0.0185 | −0.0002 | | $b_7$ | −0.0256 | 0.0014 | −0.2736 |
| $a_8$ | 0.0112 | 0.0089 | | $b_8$ | −0.0348 | 0.0018 | |
| $a_9$ | 0.0180 | 0.0109 | | | | | |

For the excitation of the $(n+1)\,^1P_1$ states in both Zn and Yb we found a simple spectroscopic configuration was adequate. Thus, the ground-state wave function was represented by a single $(ns^2)$ configuration while the excited states were given by the spectroscopic configuration wave functions:

$$(n+1)^1P(J=1) : c_1(nsn'\bar{p})_{J=1} + c_2(nsn'p)_{J=1}. \quad (3)$$

The mixing coefficients were found to be $c_1 = 0.5655$ and $c_2 = 0.8247$ for Zn and $c_1 = 0.5093$ and $c_2 = 0.8606$ for Yb from the GRASP2K code [23].

Finally, for the $5\,^1D_2$ excitation in Yb, the following set of wave functions for the ground and excited states was used

$$6\,^1S(J=0) : a_1(6s^2)_{J=0} + a_2(6s7s)_{J=0} + a_3(5\bar{d}^2)_{J=0} + a_4(5d^2)_{J=0} \quad (4)$$

and

$$5\,^1D(J=2) : b_1(5\bar{d}6s)_{J=2} + b_2(5d6s)_{J=2} + b_3(5\bar{d}^2)_{J=2} + b_4(5\bar{d}5d)_{J=2} + b_5(5d^2)_{J=2} + b_6(6s6\bar{d})_{J=2} + b_7(6s6d)_{J=2}, \quad (5)$$

whose mixing coefficients obtained from the GRASP2K code [23] are also included in Table I.

Our calculated optical oscillator strength (OOS) for the dipole-allowed transitions in Zn and Yb are given in Tables II and III. These are compared with the critically evaluated NIST values [24] as well as available experimental [25–28] and other theoretical [2,8,29–31] results as a check on the quality of our wave functions. From Table II, we observe that our calculated OOS for the $4\,^1P_1 \rightarrow 4\,^1S_0$ transition in Zn is 1.46, which matches the value given by NIST [24] and is very close to the experimental measurements [25,28] and the value obtained by the CCC calculation, that is, 1.47. The other theoretical values [29,30] are also in good agreement. For the $5\,^1P_1 \rightarrow 4\,^1S_0$ transition in Zn there are no experimental values of the OOS reported in the literature. However, our calculated value 0.089 is very close to recently reported theoretical results obtained by Zatsarinny and Bartschat [29] and Liu *et al.* [30]. The value 0.11 obtained from the CCC calculation [2] and the theoretical result 0.122 taken from [31] are somewhat higher. In Table III we observe that our calculated OOS for the $6\,^1P_1 \rightarrow 6\,^1S_0$ transition in Yb is 1.20 from GRASP2K code [23], which is in good agreement with the other theoretical and experimental results shown in the table. In contrast, our calculated OOS for the $7\,^1P_1 \rightarrow 6\,^1S_0$ transition in Yb is 0.22, which is in very good agreement with the value given by NIST [24], that is, 0.25 but much higher than the OOS obtained from the RCCC calculation [8].

The transition matrix for the electron excitation of an atomic system from initial state $|J_aM_a\rangle$ to final state $|J_bM_b\rangle$ can be expressed in the first-order RDW approximation as (atomic units are used throughout the paper)

$$T(J_b,M_b,\mu_b;J_a,M_a,\mu_a) = \langle\varphi_b(1,\ldots,N)F^-_{b,\mu_b}(k_b,N+1)|V - U|A\varphi_a(1,\ldots,N)F^+_{a,\mu_a}(k_a,N+1)\rangle, \quad (6)$$

where $J_a$, $J_b$ and $M_a$, $M_b$ are quantum numbers referring the total angular momentum and $z$ component of the bound state and $\mu_a$, $\mu_b$ are the spin projections of the projectile electron. The transition matrix contains contributions from direct excitation as well as exchange of projectile electron with the one of the valence electrons via the antisymmetrizing operator $A$. As well, $k_a$ and $k_b$ are the momenta of the incident and scattered electron while $\phi_a$ and $\phi_b$ are the wave functions of initial and final states of the target *viz*. Zn or Yb, as described above. $V$ is the interaction potential between the projectile

TABLE II. Optical oscillator strength for different transitions considered in Zn.

| Transitions | GRASP2K [23] | NIST [24] | Lurio *et al.* [28] | Doidge [25] | CCC [2] | Zatsarinny and Bartschat [29] | Liu *et al.* [30] | Verner *et al.* [31] |
|---|---|---|---|---|---|---|---|---|
| $4\,^1S_0 \rightarrow 4\,^1P_1$ | 1.46 | 1.46 | 1.46 | 1.47 | 1.47 | 1.45 | 1.514 | |
| $4\,^1S_0 \rightarrow 5\,^1P_1$ | 0.089 | | | | 0.11 | 0.095 | 0.096 | 0.122 |

TABLE III. Optical oscillator strength for different transitions considered in Yb.

| Transitions | GRASP2K [23] | NIST [24] | RCCC [8] | CCC [8] | Lange [26] | Baumann and Wandel [27] |
|---|---|---|---|---|---|---|
| $6\ ^1S_0 \rightarrow 6\ ^1P_1$ | 1.20 | 1.26 | 1.29 | 1.28 | 1.27 | 1.30 |
| $6\ ^1S_0 \rightarrow 7\ ^1P_1$ | 0.22 | 0.25 | 0.005 | | | |

electron and the target atom. The distorted waves $F^{+(-)}_{a(b),\mu_{a(b)}}$ describing the projectile electrons are the solution of the relativistic free-particle Dirac-Fock equations with outgoing (incoming) boundary conditions in the field of the distortion potential $U$, which is taken to be ground-state static potential of the atom. Once we obtain the $T$ matrix, the DCS is calculated

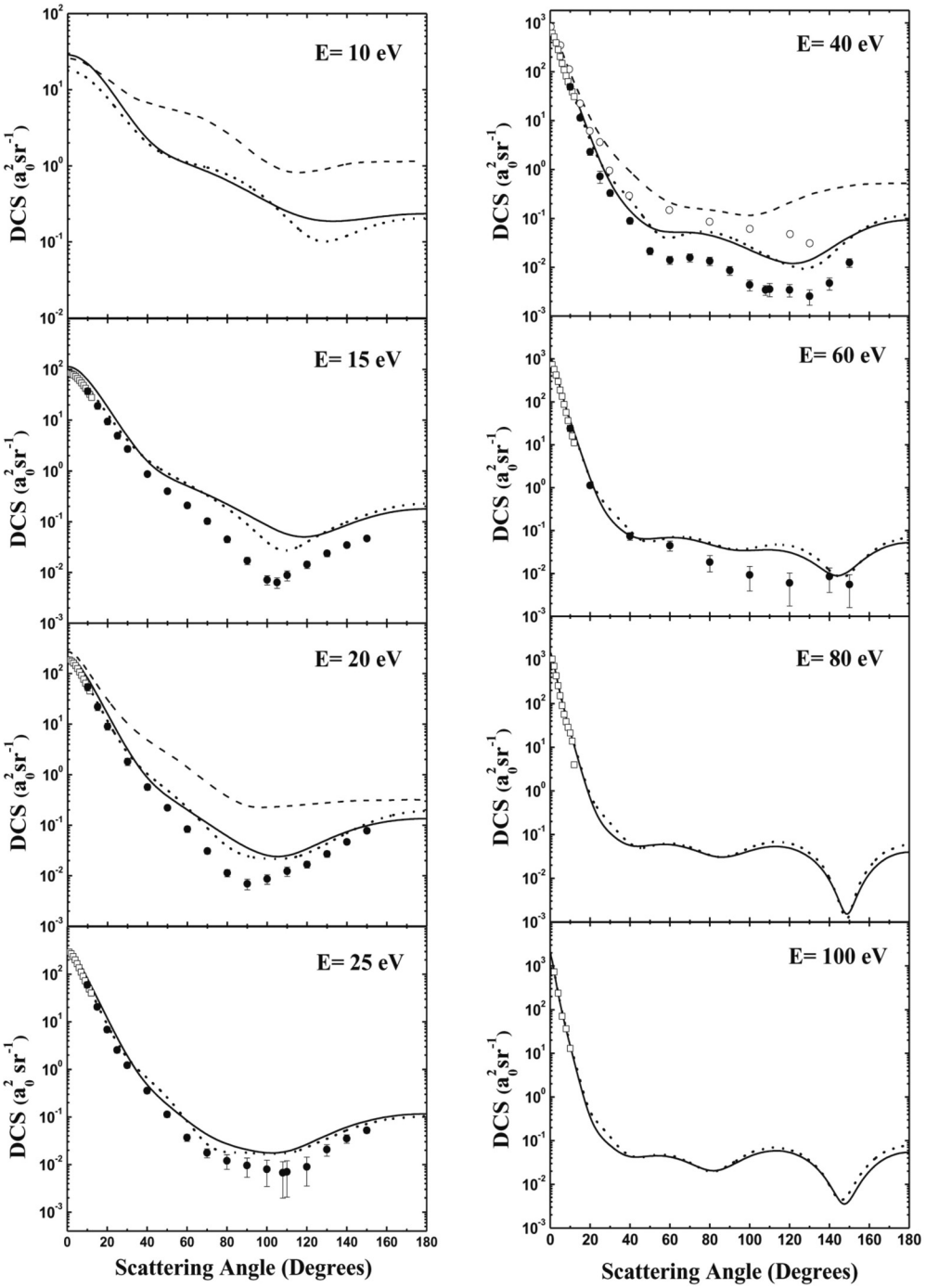


FIG. 1. Differential cross sections (DCSs) (in units of $a_0^2$ sr$^{-1}$) for electron-impact excitation of the 4 $^1P_1$ state of zinc at different incident electron energies. Theory: solid line, present RDW results; dashed line, previous RDW results [15]; dotted line, CCC calculations [2]; experiment: solid circles, Fursa *et al*. [2]; open squares, Panajotovic *et al*. [1]; open circles, Williams and Bozinis [14].

from the following formula:

$$\frac{d\sigma}{d\Omega} = (2\pi)^4 \frac{k_b}{k_a} \left| T^{\mathrm{RDW}}_{a\to b} \right|^2. \tag{7}$$

The ICS have been obtained by integrating the DCS overall scattering angles.

The bound-state wave functions calculated by the GRASP2K code [23] converge to at least one part in $10^6$, while the solution of the free-particle Dirac-Fock equations is accurate to one part in $10^5$. The accuracy of the radial integration involving these functions is governed by the accuracy of the integrands as well as the integration method used. We have accurately evaluated the oscillating long-range contribution to the direct terms in the $T$ matrix by using contour integration so the overall error in the radial integration should not exceed one part in $10^4$. In evaluating the $T$ matrix in (6) we expand the free wave functions in partial waves and calculate the individual terms for increasing values of their angular momentum until they agree with the equivalent relativistic Born term to one part in $10^5$. We then use the Born subtraction method to effectively sum this series to infinity. Thus, the overall accuracy of the results reported here is at least one part in $10^4$ within the RDW approximation used.

## III. RESULTS AND DISCUSSION

### A. Generalized oscillator strength

The generalized oscillator strength (GOS) is defined in terms of the DCS $d\sigma/d\Omega$ by the following formula [32–34]:

$$f(K,E) = \frac{\omega k_a}{2k_b} K^2 \left( \frac{d\sigma}{d\Omega} \right), \tag{8}$$

where $\omega$ is the excitation energy for the transition in atomic units, $k_a$ and $k_b$ are the initial and final momenta, respectively, of the electron, and $K$ is the momentum transfer expressed in terms of the scattering angle $\theta$ by the relation

$$K^2 = 2E \left[ 2 - \frac{\omega}{E} - 2\sqrt{\left(1 - \frac{\omega}{E}\right)} \cos\theta \right], \tag{9}$$

where $E$ is the incident electron-impact energy in atomic units. The limit of the GOS for optically allowed transitions as $K \to 0$ is the OOS. Since $K$ cannot physically reach this limit in the case of an excitation process, the resulting GOS values have to be extrapolated in order to achieve this limit. To avoid such an extrapolation, Avdonina *et al.* [32] introduced the forward-scattering function (FSF), which is the limit of the GOS when $\theta = 0$. This function depends on the value of the OOS assumed for the transition in question.

For the $4\,{}^1S_0 \to 4\,{}^1P_1$ excitation measurements in Zn, Panajotović *et al.* [1] normalized their results at small scattering angles to the FSF and the later measurements at larger scattering angles [2] have been subsequently normalized to these small-angle results. They used the experimental oscillator strength 1.47 [25] for this purpose, which is very close to the value we obtained. For the normalization of the $5\,{}^1P_1$ they used the OOS value of 0.122 [31] which is somewhat higher than our value of 0.089. Williams and Bozinis have used the value of 1.46 [28] for the oscillator strength of the $4\,{}^1S_0 \to 4\,{}^1P_1$ transition to normalize their cross sections. This normalization also determines the normalization of their cross sections for the excitation of the $5\,{}^1P_1$ state.

For Yb, the experimental DCS results of Predojević *et al.* [3] for the excitation of the $6\,{}^1P_1$ state are normalized to the FSF using a value for the OOS of 1.30 while Johnson *et al.* [16] have normalized their DCS data by utilizing the UDW ICSs at 80 eV, and then employing the optical excitation function data of Shimon *et al.* [35] to normalize their results at other energies. Predojević *et al.* [4] measured DCS for the excitation of the $(6s7p)\ {}^1P_1$ and $(5d6s)\ {}^1D_2$ relative to that for the excitation of the $6\,{}^1P_1$ state, which was normalized as described above.

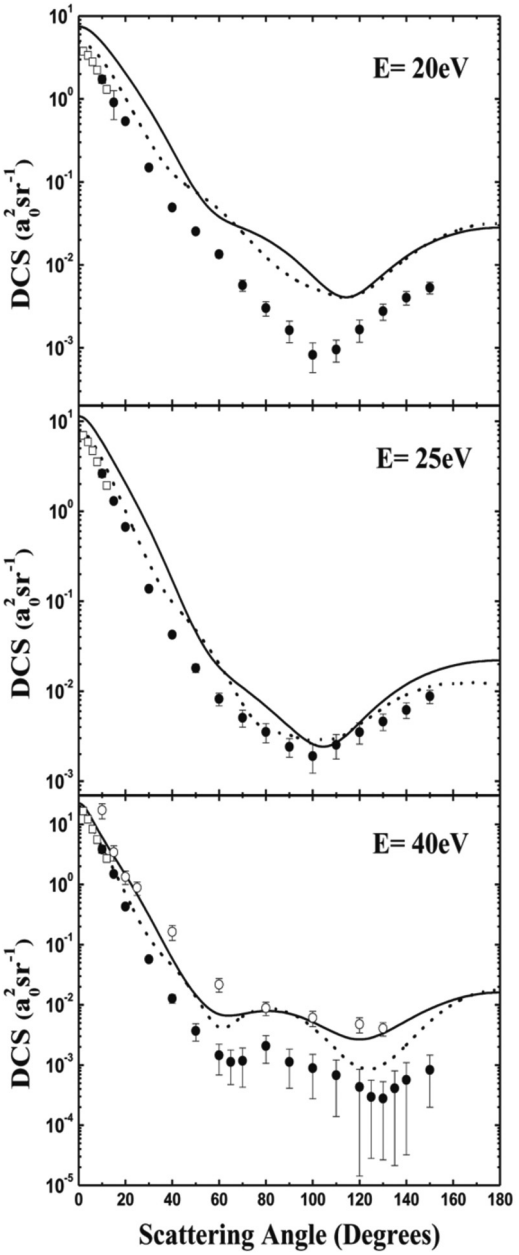


FIG. 2. As for Fig. 1 but for electron-impact excitation of the $5\,{}^1P_1$ state of zinc.

### B. Differential cross sections

#### *1. Zinc*

In Fig. 1 we present DCSs for the excitation of the 4 $^1P_1$ state of Zn from the ground state for incident electron energies from 10 to 100 eV. We have included the previous RDW calculations of Kaur *et al*. [15] at the available energies in order to access the improvement obtained by using more elaborate target wave functions. We have also included the small-angle measurements of Panajotović *et al*. [1], the measurements of Fursa *et al*. [2] in the scattering angle range up to 150°, as well as the experimental results of Williams and Bozinis [14] at 40 eV. The CCC calculations of Fursa *et al*. [2] are also included in Fig. 1 for comparison. At 10 eV energy our present RDW results are close to the CCC calculations of Fursa *et al*. [2] although somewhat larger in the forward direction. We also observe that our previous RDW calculations [15] are above the other results for all scattering angles. At 15 and 20 eV our results are much closer to the CCC calculations and the measurements of [1] in the forward direction. Although our present results and the CCC calculations agree well over the whole angular range they exceed the experimental results of [2] at intermediate and large scattering angles. As the incident energy increases to 40 eV and above, our present results become closer to the CCC values and agree very well with the small-angle DCS values of Panajotović *et al*. [1]. However, at larger scattering angles, both the CCC [2] and the present calculations tend to be higher than the measurements of Fursa *et al*. [2]. At 40 eV the measurements of Williams and Bozinis [14] are in good agreement at small scattering angles but exceed both the measurements of [2] and the CCC and present calculations at intermediate scattering angles.

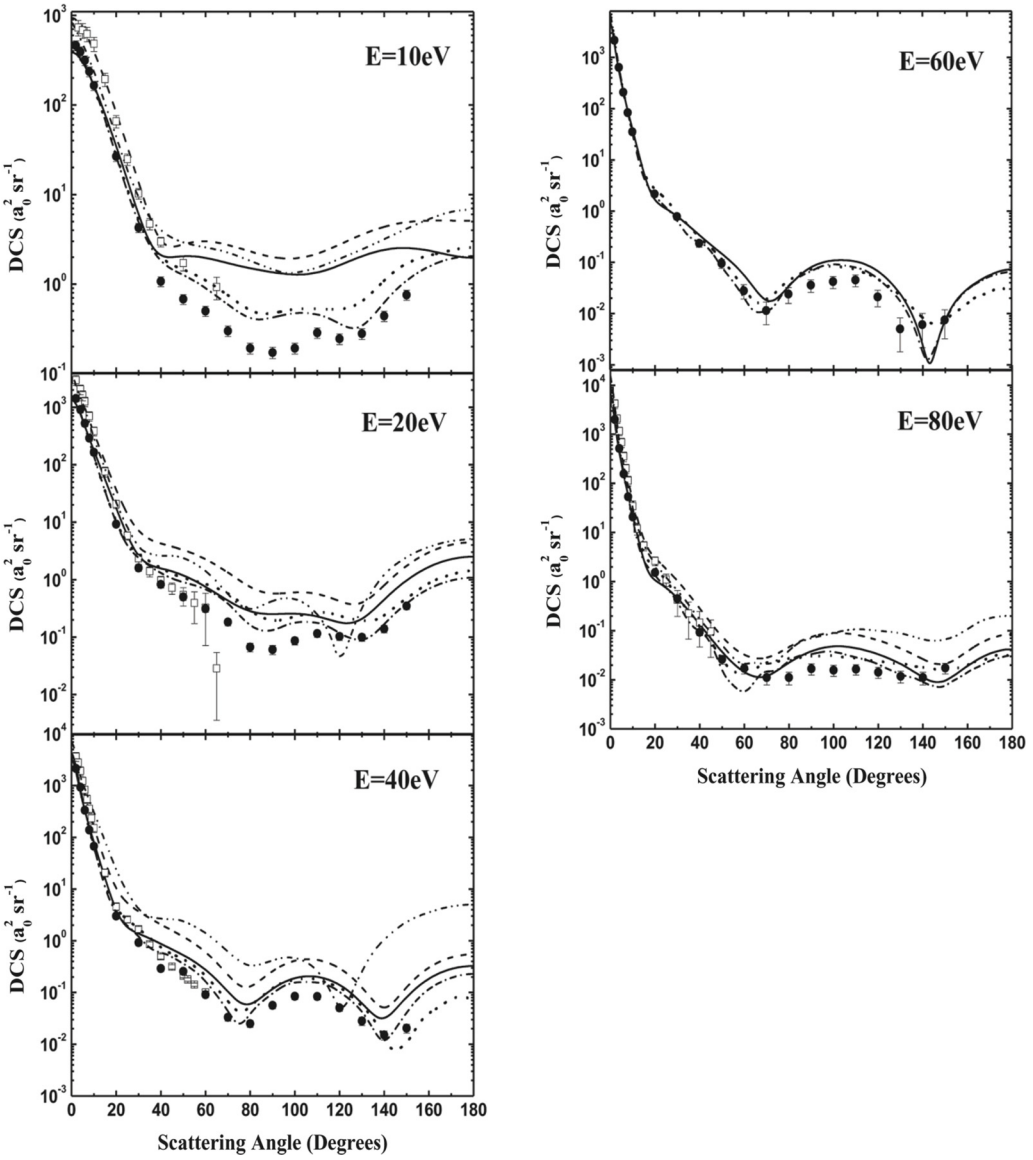


FIG. 3. Differential cross sections (DCSs) (in units of $a_0^2\,\mathrm{sr}^{-1}$) for electron-impact excitation of the 6 $^1P_1$ state of ytterbium at different incident electron energies. Theory: solid line, present RDW results; dashed line, previous RDW results [13]; dot-dashed line, RCCC calculation [8]; dotted line, CCC calculation [8]; dash-dot-dotted line,UDWA calculation [16]; experiment: solid circles, Predojevic *et al*. [3]; open squares, Johnson *et al*. [16].

In general, we find that the previous RDW results [15] are substantially higher than the present RDW calculations as well as the CCC calculations reflecting the larger OOS produced by the target-state wave functions used there.

In Fig. 2 the DCS for excitation of the 5 $^1P_1$ state at 20, 25, and 40 eV incident electron energies are presented and compared with the CCC calculations and measurements from Fursa *et al*. [2], as well as the experimental data of Panajotović *et al*. [1] and Williams and Bozinis [14]. As the energy increases, the present RDW and CCC [2] calculations converge to the low-angle measurements [1]. At 40 eV, the agreement with the experimental DCS of Williams and Bozinis [14] is quite reasonable over the entire range of scattering angles while at larger scattering angles both theoretical results are larger than the measurements of [2] at all energies.

### 2. *Ytterbium*

Figure 3 shows the DCSs for excitation of the 6 $^1P_1$ state from the ground state of ytterbium at 10, 20, 40, 60, and 80 eV incident electron energies. The present RDW calculations are compared with the experimental data of Johnson *et al*. [16] and Predejović *et al*. [3], as well as theoretical RCCC and CCC calculations from [8] and the UDWA calculations of [16,17]. In this figure we have also included the previous RDW results of Srivastava *et al*. [13]. At 10 and 20 eV the experimental data of Johnson *et al*. [16] up to 70° are seen to lie above the experimental DCS curve of Predojević *et al*. [3]. This is primarily due to the different normalization method used in obtaining the DCS results as discussed earlier. At 10 eV we find that there is good agreement among the present RDW, CCC, and RCCC calculations and the measurements of Predojević *et al*. [3] up to 40°, after which the various data sets diverge. As in Zn, the previous RDW results of [13] lie considerably higher. Above 10 eV the present RDW results are in good agreement with the CCC and RCCC calculations and measurements at small scattering angles while the discrepancies at large scattering angles becomes smaller with increasing energy of the incident electrons. The UDWA calculations also show reasonable agreement with other theories at higher energies.

Our present RDW DCS results for excitation of the 5*d*6*s* $^1D_2$ state from the ground state are presented in Fig. 4 at 10- and 20-eV incident electron energies and compared with the measurements of Predojević *et al*. [4] and the RCCC and CCC calculations [8]. At 10 eV for scattering angle up to 50° all the theoretical results agree reasonably well with the experimental data. At larger scattering angles our RDW calculations predict a larger cross section with respect to the CCC and RCCC calculations while the experimental measurement is lower by roughly the same amount. At 20 eV our RDW results are in relatively good agreement with the RCCC and CCC calculations [8] over the entire range of scattering angles. The experimental results of Predojević *et al*. [4] agree with the theoretical results up to 50° but are considerably lower for larger angles though the shape is similar to the theoretical curves.

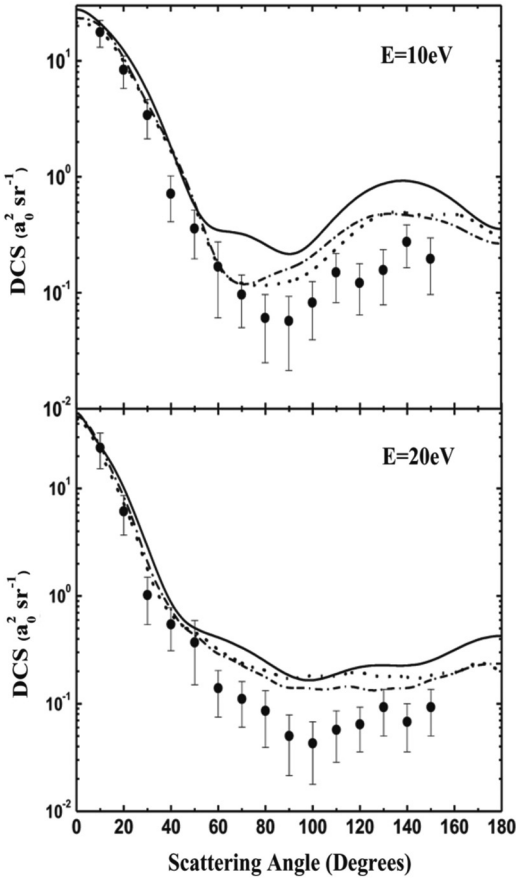


FIG. 4. As for Fig. 3 but for electron-impact excitation of the 5 $^1D_2$ state of ytterbium.

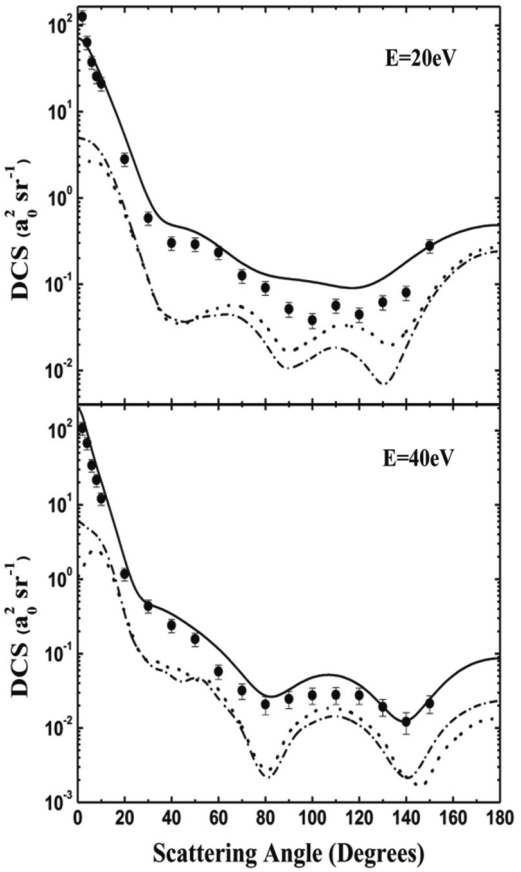


FIG. 5. As for Fig. 3 but for electron-impact excitation of the 7 $^1P_1$ state of ytterbium.

Finally, in Fig. 5 we show our present RDW calculations of the DCS for the excitation of the 7 $^1P_1$ state at 20 and 40 eV. Our results are in good agreement with the experimental results of Predejović *et al*. [4] over most of the angular range. However, both the RCCC and the CCC DCSs of [8] are significantly lower at all angles, reflecting the much smaller values of the OOS they find.

### C. Integrated cross sections

In Figs. 6 and 7, respectively, we show our ICSs for the different transitions considered in Zn and Yb. In Fig. 6 for Zn, we include the ICS obtained from the DCS measurements of [2,14] and the CCC calculations of [2] as well as those of Zatsarinny and Bartschat [29] and the measurements of Shpenik *et al*. [36] for excitation of the 4 $^1P_1$ state. We observe that the ICS results follow the general trends seen for the DCS; that is, the agreement improves with the measurements of the Belgrade group and the CCC calculations as the energy increases. The ICS of Williams and Bozinis [14] are considerably above the other results, as expected from their DCS measurements. The calculations of Zatsarinny and Bartschat [29] produce results close to those of the CCC calculations [2] while the low-energy measurements of [36] agree with the lowest-energy measurement of [2].

For the excitation of Yb, we include the ICS results obtained from the DCS measurements of [3,4,16] in Fig. 7. We have also included the CCC and RCCC results of [8], the UDWA calculations from [16], as well as our previous RDW results [13]. Reflecting the behavior of the DCS, the measurements of [16] as well as the UDWA [16] and previous RDW [13] calculations are substantially above the present results. We agree well with results obtained from the DCS measurements of [3,4] as well as the CCC and RCCC calculations [8] with the exception of the excitation of the 7 $^1P_1$ state, where the CCC and RCCC results are much lower, as we have shown for the DCS.

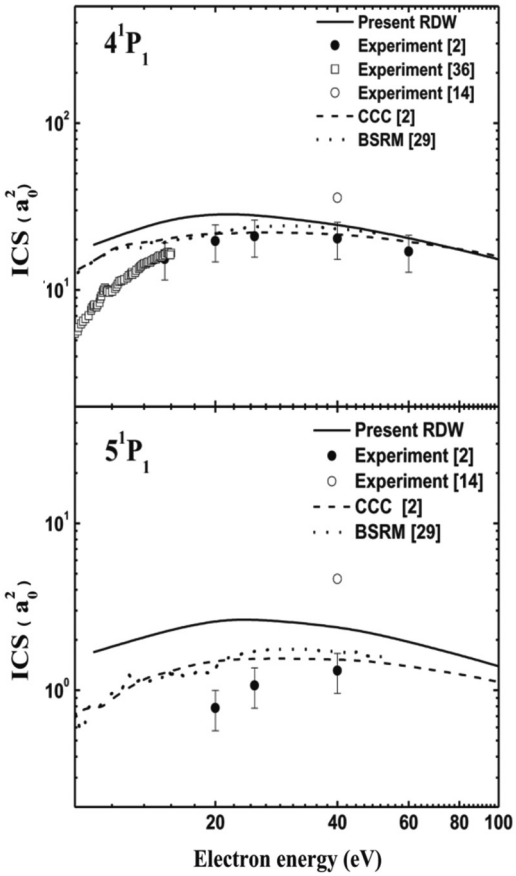


FIG. 6. Integrated cross sections (ICSs) (in units of $a_0^2$) for electron-impact excitation of the 4 $^1P_1$ and 5 $^1P_1$ states of zinc.

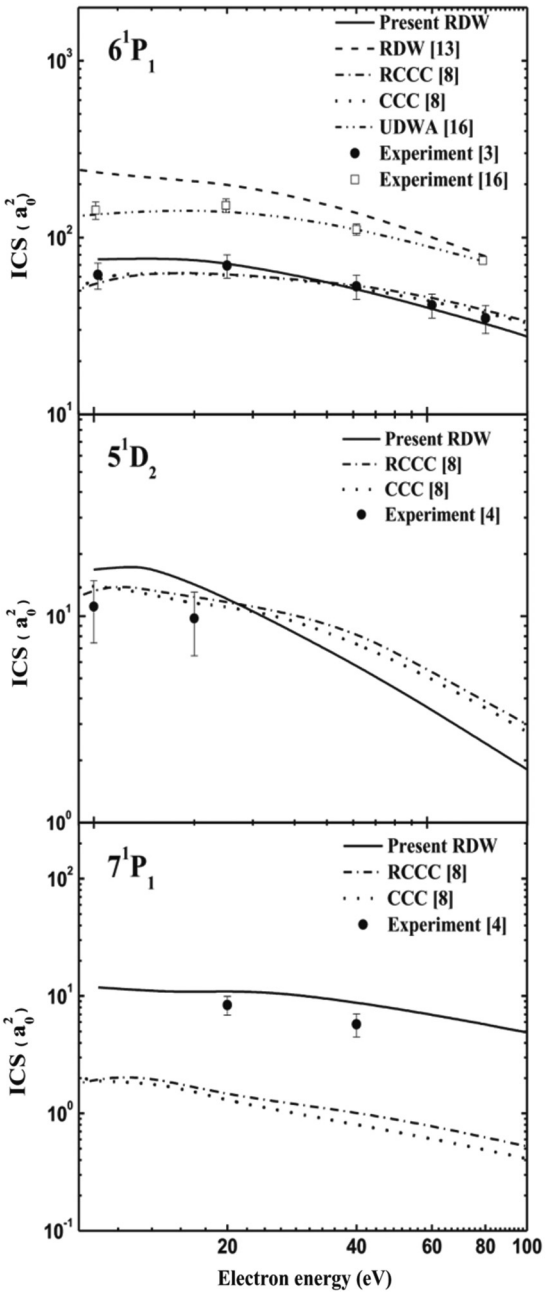


FIG. 7. Integrated cross sections (ICSs) (in units of $a_0^2$) for electron-impact excitation of the 6 $^1P_1$, 5 $^1D_2$ and 7 $^1P_1$ states of ytterbium.

## IV. CONCLUSIONS

We have used our RDW method to calculate the differential and integrated cross sections for electron-impact excitation of

the 4 $^1P_1$ and 5 $^1P_1$ in Zn and 6 $^1P_1$, 7 $^1P_1$, and 5 $^1D_2$ states in Yb from their ground states. The results are compared with the recent experimental results and theoretical CCC calculations. The use of elaborate multiconfiguration bound-state wave functions lowers our present results from our previous RDW calculated values, bringing them into significantly better agreement with the measurements of the Belgrade group and the CCC and RCCC calculations. Obtaining accurate values for the OOS is crucial in obtaining reliable DCS results for these atoms. The use of differing values of the OOS to normalize the experimental measurements contributes to the problem of comparison between theory and experiment. It is important to have accurate values for these quantities for both experimental and theoretical applications.

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[1] R. Panajotović, D. Šević, V. Pejčev, D. M. Filipović, and B. P. Marinković, Int. J. Mass Spectrom. **233**, 253 (2004).
[2] D. V. Fursa, I. Bray, R. Panajotović, D. Šević, V. Pejčev, D. M. Filipović, and B. P. Marinković, Phys. Rev. A **72**, 012706 (2005).
[3] B. Predojević, D. Šević, V. Pejčev, B. P. Marinković, and D. M. Filipović, J. Phys. B **38**, 1329 (2005).
[4] B. Predojević, D. Šević, V. Pejčev, B. P. Marinković, and D. M. Filipović, J. Phys. B **38**, 3489 (2005).
[5] J. D. Hein, S. Kidwai, P. W. Zetner, C. Bostock, D. V. Fursa, I. Bray, L. Sharma, R. Srivastava, and A. D. Stauffer, J. Phys. B **44**, 015202 (2011).
[6] J. D. Hein, S. Kidwai, P. W. Zetner, C. Bostock, D. V. Fursa, I. Bray, L. Sharma, R. Srivastava, and A. D. Stauffer, J. Phys. B **44**, 075201 (2011).
[7] L. Pravica, J. F. Williams, D. Cvejanović, S. Samarin, K. Bartschat, O. Zatsarinny, A. D. Stauffer, and R. Srivastava, Phys. Rev. A **83**, 040701 (2011).
[8] C. J. Bostock, D. V. Fursa, and I. Bray, Phys. Rev. A **83**, 052710 (2011).
[9] M. Born, J. Phys. D **34**, 909 (2001).
[10] Y. P. Zhou, J. H. Jiang, H. L. Wu, G. L. Shen, R. Q. Yu, and Y. Ozaki, J. Chemom. **20**, 13 (2006).
[11] Y. Li and P. W. Zetner, J. Phys. B **27**, L293 (1994).
[12] P. W. Zetner, P. V. Johnson, Y. Li, G. Csanak, R. E. H. Clark, and J. Abdallah Jr., J. Phys. B **34**, 1619 (2001).
[13] R. Srivastava, R. P. McEachran, and A. D. Stauffer, J. Phys. B **28**, 885 (1995).
[14] W. Williams and D. Bozinis, Phys. Rev. A **12**, 57 (1975).
[15] S. Kaur, R. Srivastava, R. P. McEachran, and A. D. Stauffer, J. Phys. B **30**, 1027 (1997).
[16] P. V. Johnson, Y. Li, P. W. Zetner, G. Csanak, R. E. H. Clark, and J. Abdallah Jr., J. Phys. B **31**, 3027 (1998).
[17] R. E. H. Clark, J. Abdallah Jr., G. Csanak, and S. P. Kramer, Phys. Rev. A **40**, 2935 (1989).
[18] R. K. Chauhan, R. Srivastava, and A. D. Stauffer, J. Phys. B **38**, 2385 (2005).
[19] R. Srivastava, R. K. Gangwar, and A. D. Stauffer, Phys. Rev. A **80**, 022718 (2009).
[20] R. K. Gangwar, L. Sharma, R. Srivastava, and A. D. Stauffer, Phys. Rev. A **81**, 052707 (2010).
[21] R. K. Gangwar, L. Sharma, R. Srivastava, and A. D. Stauffer, Phys. Rev. A **82**, 032710 (2010).
[22] I. P. Grant, Adv. Phys. **19**, 747 (1970).
[23] P. Jönsson, X. He, C. Froese Fischer, and I. P. Grant, Comput. Phys. Commun. **177**, 597 (2007).
[24] Yu. Ralchenko, A. E. Kramida, J. Reader, and NIST ASD Team, *NIST Atomic Spectra Database* (ver. 4.1.0), http://physics.nist.gov/asd [2012, July 6] (National Institute of Standards and Technology, Gaithersburg, MD, 2011).
[25] P. S. Doidge, Spectrochim. Acta, Part B **50**, 209 (1995).
[26] W. Lange, J. Luther, A. Steudel, and H. Walther, Phys. Lett. **20**, 166 (1966).
[27] M. Baumann and G. Wandel, Phys. Lett. **22**, 283 (1966).
[28] A. Lurio, R. L. deZafra, and R. J. Goshen, Phys. Rev. **134**, A1198 (1964).
[29] O. Zatsarinny and K. Bartschat, Phys. Rev. A **71**, 022716 (2005).
[30] Y. P. Liu, C. Gao, J. L. Zeng, and J. R. Shi, Astron. Astrophys. **536**, A51 (2011).
[31] D. A. Verner, P. D. Barthel, and D. Tytler, Astron. Astrophys. Suppl. Ser. **108**, 287 (1994).
[32] N. B. Avdonina, Z. Felfli, and A. Z. Msezane, J. Phys. B **30**, 2591 (1997).
[33] T. Das, R. Srivastava, and A. D. Stauffer, Phys. Lett. A **375**, 568 (2011).
[34] Z. Felfli, A. Z. Msezane, and D. Bessis, Phys. Rev. Lett. **81**, 963 (1998).
[35] L. L. Shimon, N. V. Golovchak, I. I. Garga, and I. V. Kurta, Opt. Spectrosc. **50**, 571 (1981).
[36] O. B. Shpenik, I. V. Chernyshova, and J. E. Kontros, Radiat. Phys. Chem. **68**, 277 (2001).