



Advanced Optical Metrology: Geoscience II now available

Free educational eBook

For geologists, grains and sediment are important since their study and analysis represent a powerful tool in classifying rocks or for describing a site's geomorphic setting. Characterizing the physical properties of grains, for example, is critical to determine the suitability of sediment for various uses or in the study of its geologic history. The main physical properties of grains are their size and size distribution, color, shape, and composition.

In this eBook you can find images of fascinating sand grains collected from places around the world and examined with a digital microscope. Which one of the twelve astonishing sorts of grains is your favorite?

[**Download it now**](#)

Multiconfiguration Dirac–Fock calculations of Zn K-shell radiative and nonradiative transitions

Luís Martins  | Pedro Amaro | Sofia Pessanha | Mauro Guerra | Jorge Machado | Maria Luisa Carvalho | José Paulo Santos

Laboratório de Instrumentação, Engenharia Biomédica e Física da Radiação (LIBPhys-UNL), Departamento de Física, Faculdade de Ciências e Tecnologia, FCT, Universidade Nova de Lisboa, Caparica 2829-516, Portugal

Correspondence

Luís Martins, Laboratório de Instrumentação, Engenharia Biomédica e Física da Radiação (LIBPhys-UNL), Departamento de Física, Faculdade de Ciências e Tecnologia, FCT, Universidade Nova de Lisboa, Caparica, 2829-516, Portugal.
Email: ld.martins@campus.fct.unl.pt

Funding information

FCT/MCTES/PIDDAC, Grant/Award Number: UID/FIS/04559/2013; Ações Integradas Luso-Francesas, Ação Ref. TC-08-17; Programa Pessoa 2017-2018; EMPIR, Grant/Award Number: 17FUN02 MetroMMC; FCT (Portugal), Grant/Award Numbers: PD/BD/105919/2014 and SFRH/BPD/94234/2013; FCT, Grant/Award Number: PTDC/FIS-AQM/31969/2017

Zinc K-shell radiative and radiationless transition rates are calculated using the multiconfiguration Dirac–Fock method. Correlation up to the 4p orbital is included in almost all transition rate calculations. Calculated radiative transition rates and transition probabilities are compared with Scofield's Dirac–Hartree–Slater and Dirac–Hartree–Fock calculations, presenting good agreement with the later. Radiative transition intensity ratios involving the strongest lines are compared with theoretical, experimental, and empirical-fit values. Most ratios are in close agreement with the empirical-fit values from NIST's Fundamental Parameters database. Calculated radiationless transition rates and ratios are compared with Chen et al.'s Dirac–Fock values and Safronova et al.'s Dirac–Fock values. The K-LL transition rates are overall lower than Chen et al.'s values, whereas the K-LX and K-XY transition rates are overall higher. Calculated K-LX/K-LL and K-XY/K-LL ratios are relatively close to the experimental values compared. Some calculated intensities relative to $K-L_2(^1D_2)$ are in good agreement with the experimental values, whereas others present worse agreement. The calculated fluorescence yield is higher than all theoretical, experimental, and empirical-fitted values compared, probably because the total radiationless transition rate value calculated in the present work is relatively low.

1 | INTRODUCTION

Atoms with a vacancy in an atomic inner shell relax through radiative or nonradiative transition, emitting a photon or an atomic electron, respectively. The measurements and calculations of these atomic transition rates have been the subject of many scientific works. From transition rates, important quantities can be calculated, such as transition probabilities, transition intensity ratios, and fluorescence yields. These parameters are very relevant in

various areas of physical chemistry and medical research. Transition probabilities, in specific, are tabulated in codes and software of elemental analysis and Monte Carlo simulation of atomic relaxation, which depend on the accuracy of their tabulated values. Although there are numerous calculations of atomic transition rates in literature (more frequently of the K-shell), the majority of the existing works present calculations for few selected transitions. Up until the 1970s, there were relatively few comprehensive relativistic calculations of transition rates. Such occasion changed

This is an open access article under the terms of the Creative Commons Attribution License, which permits use, distribution and reproduction in any medium, provided the original work is properly cited.

© 2019 The Authors. X-Ray Spectrometry published by John Wiley & Sons Ltd

when Scofield presented radiative rates calculated for the majority of transitions and elements, first using the Dirac–Hartree–Slater theory^[1] and later using the Dirac–Hartree–Fock theory.^[2] In the same decade, Chen et al.^[3,4] presented rates of nonradiative transition calculated for the majority of possible transitions and elements, using the Dirac–Hartree–Fock theory. Scofield’s and Chen et al.’s benchmark comprehensive calculations allowed for libraries, such as the Evaluated Atomic Data Library,^[5] to present comprehensive sets of transition probabilities, which are useful regarding simulations of atomic relaxation and other applications. In the Hartree–Slater and Dirac–Hartree–Slater methods, it is considered that each electron is affected by an average field created by all other electrons, whereas in the Hartree–Fock and Dirac–Hartree–Fock methods, the average field is represented by the Coulomb and exchange operators, J_C and K_j , such that the average potential is given as

$$V(1) = V_C(1) + V_{\text{ex}}(1), \quad (1)$$

where V_C is the Coulomb potential and V_{ex} is the exchange potential. With this inclusion, the Hartree–Fock method accounts some of the Coulomb repulsion between electrons and as generally been shown to be more accurate than those of the Hartree–Slater method. However, the Hartree–Fock approach does not fully describe the Coulomb repulsion between electrons. In fact, the major error source in this method arises from the lack of proper correlation between electrons. Thus, methods to fully account the electronic correlation have emerged, such as the multiconfiguration Hartree–Fock, configuration–interaction, many-body perturbation theory, and their relativistic versions, RCI (relativistic configuration–interaction), MCDF (multiconfiguration Dirac–Fock), RMBPT (relativistic many-body perturbation theory), respectively. In RCI (or configuration–interaction) and MCDF (or the multiconfiguration Hartree–Fock), electronic correlation is included by writing the antisymmetric wave function of the atomic system ψ as a linear combination of configuration wave functions φ , which are wave functions for different possible configuration states: $\psi(1, 2, \dots, N) = \sum_i a_i \varphi_i$, where a_i are mixing coefficients. For example, the wave function for He in the ground state can be written as

$$\psi(\text{He}) = a_1 \varphi(1s^2) + a_2 \varphi(1s^1 2p^1) + a_3 \varphi(2p^2), \quad (2)$$

where a_1 , a_2 , and a_3 are the mixing coefficients, $\varphi(1s^2)$ is the minimum configuration state function, and $\varphi(1s^1 2p^1)$ and $\varphi(2p^2)$ are extra correlations state functions. The configuration wave functions are written as a combination of one-electron orbitals.

In this work, we present Zn K-shell radiative and nonradiative transition MCDF calculations.

2 | MCDF CALCULATIONS

For this, the MCDFGME code,^[6] developed by J. P. Desclaux and P. Indelicato, was used for the calculations of Zn K-shell transition rates. It implements the multiconfiguration Dirac–Fock method including various contributions self-consistently, such as Coulomb interaction, Breit corrections, and vacuum polarizations. It also includes quantum electrodynamics contributions. One of the many capacities of the code is the calculations of radiative and radiationless transition rates and the energies of the emitted X-rays and Auger electrons. The energy and wave function for the initial configuration, the Zn with a hole in the K-shell ($1s^1 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10}$) and the energies and wave functions of all possible final configurations attained through radiative or radiationless transitions are calculated independently, including in most cases all possible extra correlation states up to the 4p orbital. From these, radiative and radiationless transition rates for all possible radiative and radiationless transitions are calculated. In the calculation of radiative transition, correlation up to the 4p orbital is included (for both the initial and final states) in all transitions, with the exception of the K–N₁ transition where in the final state ($1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^{10}$), only the selected extra correlation configurations up to the 4p orbital are included to be able to achieve convergence. Furthermore, also for the K–N₁ transition rate calculation, to achieve convergence, some orbitals are frozen during the iterative process. Due to convergence problems, several nonradiative transition rates are calculated including only

TABLE 1 Zn K-shell radiative transition rates calculated with the multiconfiguration Dirac–Fock method

| Final configuration | State | Transition rate (s ⁻¹) |
|------------------------------|-------------------------------|------------------------------------|
| 1s2 2s1 2p6 3s2 3p6 3d10 4s2 | ² S _{1/2} | 1.022E+09 |
| 1s2 2s2 2p5 3s2 3p6 3d10 4s2 | ² P _{1/2} | 3.620E+14 |
| 1s2 2s2 2p5 3s2 3p6 3d10 4s2 | ² P _{3/2} | 7.058E+14 |
| 1s2 2s2 2p6 3s1 3p6 3d10 4s2 | ² S _{1/2} | 2.140E+08 |
| 1s2 2s2 2p6 3s2 3p5 3d10 4s2 | ² P _{1/2} | 4.899E+13 |
| 1s2 2s2 2p6 3s2 3p5 3d10 4s2 | ² P _{3/2} | 9.581E+13 |
| 1s2 2s2 2p6 3s2 3p6 3d9 4s2 | ² D _{3/2} | 6.188E+10 |
| 1s2 2s2 2p6 3s2 3p6 3d9 4s2 | ² D _{5/2} | 8.958E+10 |
| 1s2 2s2 3p6 3s2 3p6 3d10 4s1 | ² S _{1/2} | 1.394E+07 |

Note. Calculations were performed with relaxed orbitals unless if “calculation notes” state that orbitals were frozen. Extra correlation state functions from the 1s orbital up to the 4p orbital were included in the calculations unless “calculation notes” present a different orbital. In that case, the calculation was performed including extra correlation wavefunctions from the 1s orbital up to the orbital presented in “calculation notes.” In the cases where no extra correlation state functions were included, “calculation notes” state that no correlation was considered. Transition rates were presented in milliatomic units: 1 milliatomic unit = $4.134 \times 10^{-13} \text{s}^{-1}$.

TABLE 2 Zn K-shell radiationless transition rates calculated with the multiconfiguration Dirac-Fock method

| Final configuration | Final State | Transition rate (s ⁻¹) | Calculation notes |
|------------------------------|-----------------------------|------------------------------------|-------------------|
| 1s2 2p6 3s2 3p6 3d10 4s2 | ¹ S ₀ | 5.796E+13 | Frozen orbitals |
| 1s2 2s1 2p5 3s2 3p6 3d10 4s2 | ¹ P ₁ | 1.514E+14 | |
| 1s2 2s1 2p5 3s2 3p6 3d10 4s2 | ³ P ₀ | 1.209E+13 | |
| 1s2 2s1 2p5 3s2 3p6 3d10 4s2 | ³ P ₁ | 4.074E+13 | |
| 1s2 2s1 2p5 3s2 3p6 3d10 4s2 | ³ P ₂ | 3.672E+13 | |
| 1s2 2s1 2p6 3s1 3p6 3d10 4s2 | ¹ S ₀ | 3.342E+13 | |
| 1s2 2s1 2p6 3s1 3p6 3d10 4s2 | ³ S ₁ | 8.490E+10 | |
| 1s2 2s1 2p6 3s2 3p5 3d10 4s2 | ¹ P ₁ | 2.168E+13 | Frozen orbitals |
| 1s2 2s1 2p6 3s2 3p5 3d10 4s2 | ³ P ₀ | 8.607E+11 | Frozen orbitals |
| 1s2 2s1 2p6 3s2 3p5 3d10 4s2 | ³ P ₁ | 9.295E+12 | Frozen orbitals |
| 1s2 2s1 2p6 3s2 3p5 3d10 4s2 | ³ P ₂ | 4.694E+12 | |
| 1s2 2s1 2p6 3s2 3p6 3d9 4s2 | ¹ D ₂ | 9.452E+10 | |
| 1s2 2s1 2p6 3s2 3p6 3d9 4s2 | ³ D ₁ | 1.576E+11 | |
| 1s2 2s1 2p6 3s2 3p6 3d9 4s2 | ³ D ₂ | 2.172E+11 | |
| 1s2 2s1 2p6 3s2 3p6 3d9 4s2 | ³ D ₃ | 4.855E+11 | |
| 1s2 2s1 2p6 3s2 3p6 3d10 4s1 | ¹ S ₀ | 1.265E+12 | 4s correlation |
| 1s2 2s1 2p6 3s2 3p6 3d10 4s1 | ³ S ₁ | 9.226E+09 | |
| 1s2 2s2 2p4 3s2 3p6 3d10 4s2 | ¹ S ₀ | 4.584E+13 | |
| 1s2 2s2 2p4 3s2 3p6 3d10 4s2 | ¹ D ₂ | 5.080E+14 | |
| 1s2 2s2 2p4 3s2 3p6 3d10 4s2 | ³ P ₀ | 2.041E+13 | |
| 1s2 2s2 2p4 3s2 3p6 3d10 4s2 | ³ P ₁ | 2.741E+11 | |
| 1s2 2s2 2p4 3s2 3p6 3d10 4s2 | ³ P ₂ | 8.379E+13 | |
| 1s2 2s2 2p5 3s1 3p6 3d10 4s2 | ¹ P ₁ | 1.015E+13 | |
| 1s2 2s2 2p5 3s1 3p6 3d10 4s2 | ³ P ₀ | 1.553E+12 | |
| 1s2 2s2 2p5 3s1 3p6 3d10 4s2 | ³ P ₁ | 1.046E+13 | |
| 1s2 2s2 2p5 3s1 3p6 3d10 4s2 | ³ P ₂ | 3.986E+12 | |
| 1s2 2s2 2p5 3s2 3p5 3d10 4s2 | ¹ S ₀ | 6.303E+12 | No correlation |
| 1s2 2s2 2p5 3s2 3p5 3d10 4s2 | ³ P ₀ | 4.801E+12 | No correlation |
| 1s2 2s2 2p5 3s2 3p5 3d10 4s2 | ¹ P ₁ | 3.159E+10 | |
| 1s2 2s2 2p5 3s2 3p5 3d10 4s2 | ³ S ₁ | 1.734E+11 | |
| 1s2 2s2 2p5 3s2 3p5 3d10 4s2 | ³ P ₁ | 3.000E+10 | |
| 1s2 2s2 2p5 3s2 3p5 3d10 4s2 | ³ D ₁ | 5.036E+10 | |
| 1s2 2s2 2p5 3s2 3p5 3d10 4s2 | ¹ D ₂ | 6.226E+13 | Frozen orbitals |
| 1s2 2s2 2p5 3s2 3p5 3d10 4s2 | ³ P ₂ | 1.361E+11 | |
| 1s2 2s2 2p5 3s2 3p5 3d10 4s2 | ³ D ₂ | 7.140E+13 | Frozen orbitals |
| 1s2 2s2 2p5 3s2 3p6 3d9 4s2 | ³ P ₀ | 2.328E+10 | |
| 1s2 2s2 2p5 3s2 3p6 3d9 4s2 | ¹ P ₁ | 4.503E+10 | |
| 1s2 2s2 2p5 3s2 3p6 3d9 4s2 | ³ P ₁ | 4.630E+10 | |
| 1s2 2s2 2p5 3s2 3p6 3d9 4s2 | ³ D ₁ | 3.602E+10 | |
| 1s2 2s2 2p5 3s2 3p6 3d9 4s2 | ¹ D ₂ | 2.262E+11 | |
| 1s2 2s2 2p5 3s2 3p6 3d9 4s2 | ³ D ₂ | 1.325E+11 | |
| 1s2 2s2 2p5 3s2 3p6 3d9 4s2 | ³ P ₂ | 6.855E+10 | |
| 1s2 2s2 2p5 3s2 3p6 3d9 4s2 | ³ F ₂ | 9.154E+11 | |
| 1s2 2s2 2p5 3s2 3p6 3d9 4s2 | ³ F ₃ | 8.005E+11 | |
| 1s2 2s2 2p5 3s2 3p6 3d9 4s2 | ¹ F ₃ | 4.683E+12 | |
| 1s2 2s2 2p5 3s2 3p6 3d9 4s2 | ³ D ₃ | 7.987E+11 | |
| 1s2 2s2 2p5 3s2 3p6 3d10 4s1 | ³ P ₁ | 6.097E+11 | 4s correlation |
| 1s2 2s2 2p5 3s2 3p6 3d10 4s1 | ³ P ₂ | 2.100E+11 | 4s correlation |
| 1s2 2s2 2p6 3p6 3d10 4s2 | ¹ S ₀ | 1.643E+12 | No correlation |
| 1s2 2s2 2p6 3s1 3p5 3d10 4s2 | ¹ P ₁ | 3.139E+12 | |
| 1s2 2s2 2p6 3s1 3p5 3d10 4s2 | ³ P ₀ | 1.014E+11 | |
| 1s2 2s2 2p6 3s1 3p5 3d10 4s2 | ³ P ₁ | 2.208E+11 | |

(Continues)

TABLE 2 (Continued)

| Final configuration | Final State | Transition rate (s ⁻¹) | Calculation notes |
|------------------------------|-----------------------------|------------------------------------|-------------------|
| 1s2 2s2 2p6 3s1 3p5 3d10 4s2 | ³ P ₂ | 1.931E+11 | |
| 1s2 2s2 2p6 3s1 3p6 3d9 4s2 | ³ D ₁ | 2.950E+10 | |
| 1s2 2s2 2p6 3s1 3p6 3d9 4s2 | ¹ D ₂ | 8.374E+09 | |
| 1s2 2s2 2p6 3s1 3p6 3d9 4s2 | ³ D ₂ | 4.356E+10 | |
| 1s2 2s2 2p6 3s1 3p6 3d9 4s2 | ³ D ₃ | 5.647E+10 | |
| 1s2 2s2 2p6 3s1 3p6 3d10 4s1 | ¹ S ₀ | 5.598E+11 | 4s correlation |
| 1s2 2s2 2p6 3s1 3p6 3d10 4s1 | ³ S ₁ | 2.709E+07 | 4s correlation |
| 1s2 2s2 2p6 3s2 3p4 3d10 4s2 | ¹ S ₀ | 9.639E+11 | |
| 1s2 2s2 2p6 3s2 3p4 3d10 4s2 | ³ P ₀ | 9.523E+10 | |
| 1s2 2s2 2p6 3s2 3p4 3d10 4s2 | ³ P ₁ | 5.749E+09 | |
| 1s2 2s2 2p6 3s2 3p4 3d10 4s2 | ³ P ₂ | 1.452E+11 | |
| 1s2 2s2 2p6 3s2 3p4 3d10 4s2 | ¹ D ₂ | 6.965E+12 | |
| 1s2 2s2 2p6 3s2 3p5 3d9 4s2 | ³ P ₀ | 2.249E+09 | |
| 1s2 2s2 2p6 3s2 3p5 3d9 4s2 | ¹ P ₁ | 3.857E+09 | |
| 1s2 2s2 2p6 3s2 3p5 3d9 4s2 | ³ P ₁ | 5.676E+09 | |
| 1s2 2s2 2p6 3s2 3p5 3d9 4s2 | ³ D ₁ | 6.186E+08 | |
| 1s2 2s2 2p6 3s2 3p5 3d9 4s2 | ³ P ₂ | 8.494E+09 | |
| 1s2 2s2 2p6 3s2 3p5 3d9 4s2 | ¹ D ₂ | 4.142E+10 | |
| 1s2 2s2 2p6 3s2 3p5 3d9 4s2 | ³ D ₂ | 2.990E+09 | |
| 1s2 2s2 2p6 3s2 3p5 3d9 4s2 | ³ F ₂ | 7.231E+10 | |
| 1s2 2s2 2p6 3s2 3p5 3d9 4s2 | ³ D ₃ | 9.771E+09 | |
| 1s2 2s2 2p6 3s2 3p5 3d9 4s2 | ¹ F ₃ | 7.691E+11 | |
| 1s2 2s2 2p6 3s2 3p5 3d9 4s2 | ³ F ₃ | 1.525E+11 | |
| 1s2 2s2 2p6 3s2 3p5 3d10 4s1 | ³ P ₀ | 1.191E+10 | 4s correlation |
| 1s2 2s2 2p6 3s2 3p5 3d10 4s1 | ¹ P ₁ | 1.224E+11 | 4s correlation |
| 1s2 2s2 2p6 3s2 3p5 3d10 4s1 | ³ P ₁ | 9.523E+10 | 4s correlation |
| 1s2 2s2 2p6 3s2 3p5 3d10 4s1 | ³ P ₂ | 3.087E+10 | 4s correlation |
| 1s2 2s2 2p6 3s2 3p6 3d8 4s2 | ¹ S ₀ | 1.015E+08 | |
| 1s2 2s2 2p6 3s2 3p6 3d8 4s2 | ³ P ₀ | 2.985E+05 | |
| 1s2 2s2 2p6 3s2 3p6 3d8 4s2 | ³ P ₁ | 6.678E+05 | |
| 1s2 2s2 2p6 3s2 3p6 3d8 4s2 | ³ P ₂ | 4.957E+07 | |
| 1s2 2s2 2p6 3s2 3p6 3d8 4s2 | ¹ D ₂ | 2.743E+08 | |
| 1s2 2s2 2p6 3s2 3p6 3d8 4s2 | ³ F ₂ | 1.553E+06 | |
| 1s2 2s2 2p6 3s2 3p6 3d8 4s2 | ³ F ₃ | 9.110E+06 | |
| 1s2 2s2 2p6 3s2 3p6 3d8 4s2 | ³ F ₄ | 3.789E+07 | |
| 1s2 2s2 2p6 3s2 3p6 3d8 4s2 | ¹ G ₄ | 3.351E+10 | |
| 1s2 2s2 2p6 3s2 3p6 3d9 4s1 | ³ D ₁ | 2.484E+09 | 4s correlation |
| 1s2 2s2 2p6 3s2 3p6 3d9 4s1 | ¹ D ₂ | 6.574E+08 | 4s correlation |
| 1s2 2s2 2p6 3s2 3p6 3d9 4s1 | ³ D ₂ | 3.465E+09 | 4s correlation |
| 1s2 2s2 2p6 3s2 3p6 3d9 4s1 | ³ D ₃ | 4.929E+09 | 4s correlation |
| 1s2 2s2 2p6 3s2 3p6 3d10 | ¹ S ₀ | 8.502E+09 | |

Note. Calculations were performed with relaxed orbitals unless if “calculation notes” state that orbitals were frozen. Extra correlation state functions from the 1s orbital up to the 4p orbital were included in the calculations unless “calculation notes” present a different orbital. In that case, the calculation was performed including extra correlation wavefunctions from the 1s orbital up to the orbital presented in “calculation notes.” In the cases where no extra correlation state functions were included, “calculation notes” state that no correlation was considered. Transition rates were presented in milliatomic units: 1 milliatomic unit = $4.134 \times 10^{-13} \text{s}^{-1}$.

the selected extra correlation configurations up to the 4p orbital. In some transitions, only the selected extra correlation configurations up to the 4s orbital are included. For the nonradiative transition between

$1s^1 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10}$ and $1s^2 2s^2 2p^6 3p^6 4s^2 3d^{10}$, no extra correlation states were included. Additionally, in many nonradiative transition rate calculations, the orbitals were frozen during the iterative process. In all calculations, Breit interaction (including its magnetic and retardation components) and vacuum polarization contributions are included in the self-consistent field method. The calculated transition rates are presented in Tables 1 and 2. From the calculated transition rates, K-shell fluorescence yield values and transition rate ratios are obtained.

3 | RESULTS

This work's radiative transition rates calculated using the multiconfiguration Dirac-Fock method are compared in Table 3 with Scofield's Dirac-Hartree-Slater^[1] and Dirac-Hartree-Fock results.^[2]

From the transition rates obtained in the present work, transition probability values are calculated. Transition probabilities are dimensionless. For a radiative transition t , its transition probability P_t is given as the ratio of the transition rate R_t and the sum of all possible radiative transition rates, as in

$$P_t = \frac{R_t}{\sum_i R_i}, \quad (3)$$

where R_i is the rate of a radiative transition i . Using this formalism, the values obtained in the present work are presented in Table 4, where they are compared with the theoretical values from Scofield's Dirac-Hartree-Slater calculations,^[1] theoretical values from Scofield's Dirac-

TABLE 3 Radiative transition rates from this work's MCDF calculations, Scofield's Dirac-Hartree-Slater calculations,^[1] and Scofield's Dirac-Hartree-Fock calculations^[2]

| Radiative transition | HS ^[1] | HF ^[2] | MCDF |
|----------------------|-------------------|-------------------|-----------|
| K-L ₁ | 2.07E-05 | n.p. | 2.473E-05 |
| K-L ₂ | 8.282 | 8.591 | 8.756 |
| K-L ₃ | 16.1 | 16.7 | 17.07 |
| K-M ₁ | 4.08E-06 | n.p. | 5.176E-06 |
| K-M ₂ | 1.024 | 1.17 | 1.185 |
| K-M ₃ | 2.00 | 2.29 | 2.318 |
| K-M ₄ | 1.39E-03 | n.p. | 1.497E-03 |
| K-M ₅ | 2.00E-03 | n.p. | 2.167E-03 |
| K-N ₁ | 2.46E-07 | n.p. | 3.362E-07 |
| Total | 27.4 | 29.0 | 29.33 |

Note. Values not presented in their references are presented in the table as "n.p." All values are presented in milliatomic units: 1 milliatomic unit = $4.134 \times 10^{-13} \text{ s}^{-1}$

TABLE 4 Radiative transition probabilities obtained from this work's MCDF calculations, Scofield's Dirac-Hartree-Slater calculations,^[1] Scofield's Dirac-Hartree-Fock calculations,^[2] and NIST's Fundamental Parameters Database^[7]

| P_t | MCDF | HS ^[1] | HF ^[2] | NIST ^[7] |
|--------------------|-----------|-------------------|-------------------|---------------------|
| K-L ₁ | 8.429E-07 | 7.538E-07 | n.p. | 3.16E-04 |
| K-L ₂ | 0.298 | 0.302 | 0.299 | 0.294 |
| K-L ₃ | 0.582 | 0.588 | 0.581 | 0.576 |
| K-M ₁ | 1.76E-07 | 1.49E-07 | n.p. | n.p. |
| K-M ₂ | 0.040 | 0.037 | 0.041 | 0.044 |
| K-M ₃ | 0.079 | 0.073 | 0.080 | 0.085 |
| K-M ₄ | 5.10E-05 | 5.05E-05 | n.p. | n.p. |
| K-M ₅ | 7.39E-05 | 7.30E-05 | n.p. | n.p. |
| K-M _{4,5} | 1.25E-04 | 1.23E-04 | n.p. | 8.16E-04 |
| K-N ₁ | 1.15E-08 | 8.96E-09 | n.p. | n.p. |

Note. Values that could not be obtained, because transition rates were not presented in their references, are presented in the table as "n.p."

Hartree-Fock calculations,^[2] and the empirical values present in NIST's Fundamental Parameters Database.^[7] The transition probability values presented in NIST's Fundamental Parameters Database^[7] are obtained from empirical fitting functions to Salem et al.'s collection of K-shell experimental transition intensity ratios^[8] and some treatment to the data to convert from transition ratios to transition probabilities. It is worthwhile mentioning that Salem et al.'s collection^[8] is still to this date the most complete source of experimental X-ray transition intensity ratios, in what concerns K-shell and L-shell transitions. Although Scofield's Hartree-Fock reference^[2] does not present transition rates for the K-L₁, K-M₁, K-M₄, K-M₅, and K-N₁ transitions, these values can be considered negligible when comparing with the sum of all possible radiative transition rates; thus, transition probabilities obtained from the Hartree-Fock rates are calculated (from Equation 3) using only the K-L₂, K-L₃, K-M₂, and K-M₃ transitions. NIST's Fundamental Parameters Database does not present transition probability values for K-M₁, K-M₄, K-M₅, and K-N₁ transitions, although it presents values for K-M_{4,5} transition, which is equivalent to the sum of K-M₄ and K-M₅ values.

Radiative transition ratios obtained from this work's multiconfiguration Dirac-Fock calculations are compared in Table 5 with ratios obtained from Scofield's Dirac-Hartree-Slater calculations,^[1] Scofield's Dirac-Hartree-Fock calculations,^[2] and the empirical-fit values from NIST's Fundamental Parameters Database.^[7] The designations for the transitions used in Table 5 are presented in Table 6. Because there is in literature a large quantity of experimental and theoretical results for $K\beta/K\alpha$ intensity ratio, we present these values in a separate table (Table 7

TABLE 5 Radiative transition ratios obtained from this work's MCDF calculations, Scofield's Dirac–Hartree–Slater calculations,^[1] and Scofield's Dirac–Hartree–Fock calculations,^[2] empirical fit values from NIST's Fundamental Parameters Database, and Salem et al.'s^[8] empirical fit values

| Transition | | | | | |
|-----------------------|----------|-------------------|-------------------|---------------------|----------------------|
| intensity ratio | MCDF | HS ^[1] | HF ^[2] | NIST ^[7] | Salem ^[8] |
| $K\alpha_2/K\alpha_1$ | 0.513 | 0.514 | 0.5142 | 0.511 | 0.510 |
| $K\beta_3/K\beta_1$ | 0.511 | 0.511 | 0.5108 | 0.518 | n.p. |
| $K\beta_1'/K\alpha_1$ | 0.205 | 0.1879 | 0.2135 | 0.224 | n.p. |
| $K\beta_2'/K\alpha_1$ | 1.97E–08 | 1.53E–08 | n.p. | n.p. | n.p. |
| $K\alpha_3/K\alpha_1$ | 1.45E–06 | 1.28E–06 | n.p. | 5.49E–04 | n.p. |
| $K\beta_1/K\alpha_1$ | 0.136 | 0.1242 | 0.137 | 0.147 | n.p. |
| $K\beta_5/K\beta_1$ | 1.58E–03 | 1.691E–03 | n.p. | 9.64E–03 | n.p. |

Note. Values that could not be obtained due to lack of information in their respective references are presented in the table as “n.p.”

TABLE 6 Indication of transitions corresponding to the line designations

| | |
|-------------|-------------------------------------|
| $K\alpha$ | All K-L transition |
| $K\alpha_1$ | K-L ₃ |
| $K\alpha_2$ | K-L ₂ |
| $K\alpha_3$ | K-L ₁ |
| $K\beta_1$ | K-M ₃ |
| $K\beta_3$ | K-M ₂ |
| $K\beta_5$ | K-M ₄ + K-M ₅ |
| $K\beta_1'$ | All K-M transitions |
| $K\beta_2'$ | K-N and all higher shells |
| $K\beta$ | K-M and all higher shells |

). In this table, the present work values are compared with other theoretical values, experimental values, and values obtained from empirical fittings to the experimental values. The theoretical values are those obtained from Scofield's Dirac–Hartree–Slater calculations,^[1] Scofield's Dirac–Hartree–Fock calculations,^[2] Kup et al.'s Dirac–Hartree–Fock calculations.^[9] The experimental values presented are from several works from 2001 to 2011.^[10–19] In Table 7, the values obtained through empirical fittings to the experimental data are those of Salem et al.,^[8] NIST's Fundamental Parameters Database,^[7] and Kahoul et al.^[20] Salem et al.'s fittings use experimental data up to 1974. NIST's Fundamental Parameters Database uses the same data as Salem et al., but because NIST's database only presents the radiative transition probabilities and not the ratios, we obtained them by calculating the ratios of the respective transition probabilities. Kahoul et al. use

TABLE 7 Radiative transition $K\beta/K\alpha$ ratios from several references

| | | $K\beta/K\alpha$ | |
|------------------------------------|---------------------------------|---------------------------------|-----------------|
| Theoretical | MCDF | 0.136 | |
| | Scofield (HS) ^[1] | 0.1241 | |
| | Scofield (HF) ^[2] | 0.141 | |
| | Kup et al. (HF) ^[9] | 0.136 | |
| | Ertuğrul et al. ^[10] | 0.136 ± 0.01 | |
| | Sogut et al. ^[11] | 0.1254 ± 0.0102 | |
| | Ertugrul ^[12] | 0.158 ± 0.005 | |
| | Öz ^[13] | 0.141 ± 0.01 | |
| | Experimental | Han et al. ^[14] | 0.126 ± 0.01 |
| | | Cevik et al. ^[15] | 0.136 ± 0.005 |
| | | Ertuğral et al. ^[16] | 0.1379 ± 0.005 |
| Yalçın ^[17] | | 0.1225 ± 0.0007 | |
| Yalçın ^[17] | | 0.1267 ± 0.0011 | |
| Kup Aylikci et al. ^[18] | | 0.12 ± 0.0061 | |
| Kup Aylikci et al. ^[19] | | 0.12 ± 0.0061 | |
| Empirical fit (1974–) | | Salem et al. ^[8] | 0.138 |
| Empirical fit (1974–) | | NIST ^[7] | 0.148 |
| Empirical fit (2001–2011) | | Kahoul et al. ^[20] | 0.1285 ± 0.0051 |

experimental values from the period 2001–2011 (these experimental values are also presented in Table 7).

Nonradiative transition rates are compared in Table 8 with Chen et al.'s Dirac–Hartree–Fock values^[3] and with Safronova et al.'s Dirac–Hartree–Fock values.^[21] In this table, transitions are grouped according with the holes in the shells in order to help the readability. The K-LX and K-LL transition rates and the (K-LX)/(K-LL) and (K-XY)/(K-LL) ratios are compared in Table 9 with Chen et al.'s Dirac–Hartree–Fock values,^[3] Safronova et al.'s Dirac–Hartree–Fock values,^[21] and experimental values from Bellicard et al.^[22] This work's ratios of radiationless transitions intensity relative to the $K-L_2L_3(^1D_2)$ transition are presented in Table 10, where they are compared with experimental results from Freedman et al.^[23]

From this work's calculated radiative and radiationless transition rates (presented in Tables 1 and 2), the Zn K-shell fluorescence yield value is calculated using the following equation:

$$\omega_K = \frac{A_K^{(TR)}}{A_K^{(TR)} + A_K^{(TA)}}, \quad (4)$$

where $A_K^{(TR)}$ is the total radiative transition rate, which is given by summing the rates of all possible radiative transitions filling the K-shell vacancy (presented in Table 1), and $A_K^{(TA)}$ is the total radiationless transition rate, which

TABLE 8 Nonradiative transitions rates from this work's MCDF calculations, Chen et al.'s Dirac–Hartree–Fock calculations,^[3] and Safronova et al.'s Dirac–Hartree–Fock calculations^[21]

| Nonradiative transition | Nonradiative transition (1s n1 n2) | Safronova ^[21] | Chen ^[3] | MCDF |
|--|------------------------------------|---------------------------|---------------------|--------|
| K-L ₁ L ₁ | 1s 2s 2s | 1.817 | 2.084 | 1.402 |
| K-L ₁ L ₂ + K-L ₁ L ₃ | 1s 2s 2p | 5.918 | 6.423 | 5.829 |
| K-L ₁ M ₁ | 1s 2s 3s | 0.490 | 0.564 | 0.811 |
| K-L ₁ M ₂ + K-L ₁ M ₃ | 1s 2s 3p | 0.764 | 0.840 | 0.883 |
| K-L ₁ M ₄ + K-L ₁ M ₅ | 1s 2s 3d | 0.031 | 0.040 | 0.023 |
| K-L ₁ N ₁ | 1s 2s 4s | n.p. | 0.043 | 0.031 |
| K-L ₂ L ₂ + K-L ₂ L ₃ + K-L ₃ L ₃ | 1s 2p 2p | 14.643 | 15.511 | 15.927 |
| K-L ₂ M ₁ + K-L ₃ M ₁ | 1s 2p 3s | 0.687 | 0.741 | 0.633 |
| K-L ₂ M ₂ + K-L ₂ M ₃ + K-L ₃ M ₂ + K-L ₃ M ₃ | 1s 2p 3p | 3.299 | 3.501 | 3.512 |
| K-L ₂ M ₄ + K-L ₂ M ₅ + K-L ₃ M ₄ + K-L ₃ M ₅ | 1s 2p 3d | 0.247 | 0.319 | 0.188 |
| K-L ₂ N ₁ + K-L ₃ N ₁ | 1s 2p 4s | n.p. | 0.055 | 0.047 |
| K-M ₁ M ₁ | 1s 3s 3s | 0.033 | 0.038 | 0.044 |
| K-M ₁ M ₂ + K-M ₁ M ₃ | 1s 3s 3p | 0.089 | 0.097 | 0.088 |
| K-M ₁ M ₄ + K-M ₁ M ₅ | 1s 3s 3d | 0.003 | n.p. | 0.003 |
| K-M ₁ N ₁ | 1s 3s 4s | n.p. | 0.006 | 0.014 |
| K-M ₂ M ₂ + K-M ₂ M ₃ + K-M ₃ M ₃ | 1s 3p 3p | 0.187 | 0.194 | 0.198 |
| K-M ₂ M ₄ + K-M ₂ M ₅ + K-M ₃ M ₄ + K-M ₃ M ₅ | 1s 3p 3d | 0.023 | 0.020 | 0.026 |
| K-M ₂ N ₁ + K-M ₃ N ₁ | 1s 3p 4s | n.p. | 0.008 | 0.006 |
| K-M ₄ M ₄ + K-M ₄ M ₅ + K-M ₅ M ₅ | 1s 3d 3d | n.p. | n.p. | 0.001 |
| K-M ₄ N ₁ + K-M ₅ N ₁ | 1s 3d 4s | n.p. | | 0.000 |
| Total | | 28.231 | 30.484 | 29.665 |

Note. Values not presented in their references are presented in table as “n.p.” Chen et al.^[3] do not present values for K-M₂M₂, K-M₂M₄, and K-M₂M₅ transitions. All values are presented in milliatomic units: 1 milliatomic unit = $4.134 \times 10^{-13} \text{s}^{-1}$.

is given by summing the rates of all possible radiationless

TABLE 9 Nonradiative K-LL, K-LX, and K-XY transition rates from this work's MCDF calculations, Chen et al.'s Dirac–Hartree–Fock calculations^[3], and Safronova et al.'s Dirac–Hartree–Fock calculations^[21]

| Nonradiative transitions | Safronova ^[21] | Chen ^[3] | MCDF | Experimental ^[22] |
|--------------------------|---------------------------|---------------------|--------|------------------------------|
| K-LL | 22.378 | 24.018 | 23.157 | |
| K-LX | 5.518 | 6.103 | 6.128 | |
| K-XY | 0.335 | 0.363 | 0.380 | |
| K-LX/K-LL | 0.247 | 0.254 | 0.265 | 0.30 ± 0.02 |
| K-XY/K-LL | 0.015 | 0.015 | 0.016 | 0.019 ± 0.005 |

Note. The K-LX/K-LL and K-XY/K-LL nonradiative transition ratios are from this work's MCDF calculations, Chen et al.'s Dirac–Hartree–Fock calculations,^[3] Safronova et al.'s Dirac–Hartree–Fock calculations,^[21] and experimental values from Bellicard et al.^[22] Transition rates are presented in milliatomic units: 1 milliatomic unit = $4.134 \times 10^{-13} \text{s}^{-1}$.

TABLE 10 Nonradiative transition intensity relative to K-L₂L₃ (¹D₂)

| Relative intensity transition | MCDF | Experimental ^[23] |
|---|-------|------------------------------|
| K-L ₁ L ₁ (¹ S ₀) | 0.114 | 0.058 |
| K-L ₁ L ₂ (¹ P ₁) | 0.298 | 0.28 |
| K-L ₁ L ₂ (³ P ₀) | 0.024 | <0.03 |
| K-L ₁ L ₃ (³ P ₁) | 0.080 | 0.046 |
| K-L ₁ L ₃ (³ P ₂) | 0.072 | <0.02 |
| K-L ₂ L ₂ (¹ S ₀) | 0.090 | <0.1 |
| K-L ₂ L ₃ (¹ D ₂) | 1.000 | 1.000 |
| K-L ₃ L ₃ (³ P ₀) | 0.040 | 0.04 |
| K-L ₃ L ₃ (³ P ₂) | 0.165 | 0.2 |

Note. Values presented are from this work's MCDF calculations and experimental values from Freedman et al.^[23]

TABLE 11 Comparison of K-shell fluorescence yield values from several works

| | | ω_K |
|---------------|------------------------------------|---------------|
| Theoretical | MCDF | 0.497 |
| | EADL ^[24] | 0.466 |
| | HF ^[4] | 0.488 |
| | Kup ^[9] | 0.485 |
| Experimental | Şimşek et al. ^[25] | 0.482 ± 0.022 |
| | Durak and Özdemir ^[26] | 0.482 ± 0.032 |
| | Ertugrul ^[12] | 0.460 ± 0.013 |
| | Şimşek et al. ^[27] | 0.488 ± 0.021 |
| | Gudennavar et al. ^[28] | 0.464 ± 0.010 |
| | Yashoda et al. ^[29] | 0.471 ± 0.018 |
| | Han et al., 2007 ^[14] | 0.477 ± 0.038 |
| | Aylikci et al. ^[18] | 0.485 ± 0.024 |
| | Aylikci et al. ^[18] | 0.460 ± 0.023 |
| | Aylikci et al. ^[18] | 0.459 ± 0.023 |
| | Aylikci et al. ^[18] | 0.458 ± 0.023 |
| | Aylikci et al. ^[18] | 0.467 ± 0.023 |
| | Ménesguen and Lépy ^[30] | 0.495 ± 0.022 |
| | Söğüt ^[31] | 0.525 ± 0.050 |
| Empirical fit | Bambynek ^[32] | 0.479 |
| | Krause ^[33] | 0.474 |
| | Bambynek ^[34] | 0.486 |
| | NIST ^[7] | 0.469 |
| | Kahoul et al. ^[20] | 0.463 |
| | Daoudi et al. ^[35] | 0.473 |

transitions filling the K-shell vacancy (presented in Table 2). The present's work K-shell fluorescence yield is compared in Table 11, with other values obtained from theoretical calculations (POR REFS!!!!), experimental measurements (POR REFS!!!!), and empirical fittings to experimental values (POR REFS!!!!). The theoretical values are from EADL (Evaluated Atomic Data Library),^[24] Chen et al.'s Dirac–Hartree–Fock calculations,^[4] and Kup et al.'s Dirac–Hartree–Fock calculations.^[9] The experimental values are from several works from 2000 to 2010.^[12,14,18,25–31] The empirical fitting values are from several works.^[7,20,32–35]

4 | CONCLUSIONS

The multiconfiguration Dirac–Fock method calculations of Zn K-shell transition rates are performed. From these values, fluorescence yield, radiative transition probabilities, and transition intensity ratios are derived and compared with theoretical and experimental values. As

presented in Table 3, radiative transition rates are in good agreement with Scofield's relativistic Dirac–Fock values.^[2] As a consequence, as presented in Table 2, radiative transition probabilities are also in good agreement with Scofield's values. This work's MCDF transition probabilities for the K-L₂, K-L₃, K-M₂, and K-M₃ transitions are in close agreement with the empirical values from NIST's Fundamental Parameters Database,^[7] whereas for the K-L₁ and K-M_{4,5} transitions, the same cannot be said.

As for radiative transition ratios, as presented in Table 5, this work's values are in good agreement with Scofield's Hartree–Fock values.^[2] When comparing against NIST's database ratios,^[7] relatively good agreement is presented for the $K\alpha_2/K\alpha_1$, $K\beta_3/K\beta_1$, and $K\beta_1'/K\alpha_1$ ratios, but strong disagreement is found for the $K\alpha_3/K\alpha_1$ and $K\beta_5/K\beta_1$ ratios.

From the comparison of $K\beta/K\alpha$ ratios, presented in Table 7, it is interesting that Kup et al.^[9]'s value is equal to the present work's MCDF value, even though in their calculations, no multiconfiguration wavefunctions were included except those of intermediate coupling. When comparing the present work's MCDF value with the theoretical values from Scofield, closer agreement is found with Scofield's Dirac–Hartree–Fock value.^[2] Even though NIST's Fundamental Parameters Database^[7] uses Salem et al.'s ratios,^[8] their value differ from one another. This discrepancy can be due to NIST's database treatment to Salem et al.'s data. The present work value is in good agreement with Salem et al.'s empirical fit value^[8] and with Kahoul et al.'s empirical fit value.^[20]

As presented in Table 8, this work's values of radiationless transition rates are often lower than Chen et al.'s^[3] values and often higher than Safronova et al.'s values.^[21] It is presented in Table 9 that the K-LL total value is lower than Chen et al.'s value and higher than Safronova. As for the K-LX and K-XY total rates, these presented values are higher than the other compared. Thus, the K-LX/K-LL and K-XY/K-LL ratios from this work are higher than the other values compared. The nonradiative transition intensities relative to the K-L₂(¹D₂) transition, as presented in Table 10, are in most cases in good agreement with the experimental results presented.

The fluorescence yield value from this work is higher than all other theoretical and experimental values compared in Table 11. It is likely that the total radiationless transition rate $A^{(TA)}$ calculated in the present work is lower than it should be, and as a result, the K-shell fluorescence yield is calculated higher than it should be (as can be seen from Equation 4). Such is supported by the comparisons in Table 9, where it is shown that the calculated value for the total K-LL transitions rate is lower than the value from Chen et al.'s calculations.^[3] Interestingly, the most recent values obtained through empirical fittings, which are those

of Daoudi et al. and Kahoul et al., are significantly lower than all the theoretical values, with the exception of values from EADL, which are the only theoretical values calculated using the Dirac–Hartree–Slater method, instead of the Dirac–Hartree–Fock method.

ACKNOWLEDGEMENTS

This work was supported by the research center grant UID/FIS/04559/2013 to LIBPhys-UNL, from the FCT/MCTES/PIDDAC, Portugal. J. P. S. and J. M. acknowledge the support of the “Ações Integradas Luso-Francesas, Ação Ref. TC-08-17, financed by the CRUP (Portugal) and CPU (France) and the “Programa Pessoa 2017-2018,” Proc. N 441.00 France, financed by the FCT (Portugal) and PHC (France). J. M. acknowledges the support of EMPiR, under Contract No. 17FUN02 MetroMMC. The EMPiR initiative is cofunded by the European Union's Horizon2020 research and innovation programme and the EMPiR participating States. L. M. and S. P. acknowledge the support of FCT (Portugal) under Contracts No. PD/BD/105919/2014 and No. SFRH/BPD/94234/2013. M. G. acknowledges the support of the FCT, under the project PTDC/FIS_x2010/AQM/31969/2017, “Ultra-high-accuracy X-ray spectroscopy of transition metal oxides and rare earths.”

ORCID

Luis Martins  <https://orcid.org/0000-0003-4815-022X>

REFERENCES

- [1] J. H. Scofield, *At. Data Nucl. Data Tables* **1974a**, 14(2), 121.
- [2] J. Scofield, *Phys. Rev. A* **1974b**, 9(3), 1041.
- [3] M. H. Chen, B. Crasemann, H. Mark, *At. Data Nucl. Data Tables* **1979**, 24(1), 13.
- [4] M. H. Chen, B. Crasemann, H. Mark, *Phys. Rev. A* **1980**, 21(2), 436.
- [5] D. Cullen, S. T. Perkins, D. E. Cullen, M. H. Chen, J. H. Hubbell, J. Rathkopf, J. Scofield, Tables and Graphs of Atomic Subshell and Relaxation Data Derived from the LLNL Evaluated Atomic Data Library (EADL), $Z = 1 - 100$, **1991**.
- [6] J. P. Desclaux, *Comput. Phys. Commun.* **1975**, 9(1), 31.
- [7] W. T. Elam, B. D. Ravel, J. R. Sieber, *Radiat. Phys. Chem.* **2002**, 63(2), 121.
- [8] S. I. Salem, S. L. Panossian, R. A. Krause, *At. Data Nucl. Data Tables* **1974**, 14(2), 91.
- [9] N. Kup Aylikci, J. M. Sampaio, A. Kahoul, V. Aylikci, I. H. Karahan, M. Guerra, J. P. Santos, J. P. Marques, E. Tiraşoğlu, *X-Ray Spectrom.* **2017**, 46(4), 242.
- [10] M. Ertugrul, Ö. Sögüt, Ö. Simsek, E. Büyükkasap, *J. Phys. B Atomic Mol. Phys.* **2001**, 34(5), 909.
- [11] O. Sogut, E. Büyükkasap, H. Erdoğan, *Radiat. Phys. Chem.* **2002**, 64(5-6), 343.
- [12] M. Ertugrul, *Anal. Chim. Acta* **2002**, 454(2), 327.
- [13] E. Öz, *J. Quant. Spectrosc. Radiat. Transf.* **2006**, 97(1), 41.
- [14] I. Han, M. Şahin, L. Demir, Y. Şahin, *Appl. Radiat. Isot.* **2007**, 65(6), 669.
- [15] U. Cevik, S. Kaya, B. Ertugral, H. Baltas, S. M. Karabidak, *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* **2007**, 262(2), 165.
- [16] B. Ertuğral, G. Apaydin, U. Çevik, M. Ertuğrul, A.İ. Kobya, *Radiat. Phys. Chem.* **2007**, 76(1), 15.
- [17] P. Yalçun, *Nucl. Instrum. Methods Phys. Res., Sect. B* **2007**, 254(2), 182.
- [18] N. K. Aylikci, E. Tiraşoğlu, H. Karahan, V. Aylikci, E. Cengiz, G. Apaydin, *Chem. Phys. Lett.* **2010**, 484(4-6), 368.
- [19] N. Kup Aylikci, V. Aylikci, A. Kahoul, E. Tiraşoğlu, H. Karahan, E. Cengiz, *Phys. Rev. A* **2011**, 84(4), 42509.
- [20] A. Kahoul, V. Aylikci, N. Kup. Aylikci, E. Cengiz, G. Apaydin, *Radiat. Phys. Chem.* **2012**, 81(7), 713.
- [21] U. I. Safronova, W. R. Johnson, J. R. Albritton, *At. Data Nucl. Data Tables* **2001**, 77(2), 215.
- [22] J. B. Bellicard, A. Moussa, S. K. Haynes, *Nucl. Phys.* **1957**, 3(2), 307.
- [23] M. S. Freedman, F. T. Porter, F. Wagner, *Phys. Rev.* **1966**, 151(3), 886.
- [24] S. T. Perkins, D. E. Cullen, M. H. Chen, J. Rathkopf, J. Scofield, J. H. Hubbell, United States: N. p., 1991. Web. <https://doi.org/10.2172/10121422>.
- [25] Ö. Şimşek, O. Doğan, Ü. Turgut, M. Ertuğrul, *Radiat. Phys. Chem.* **2000**, 58(3), 207.
- [26] R. Durak, Y. Özdemir, *Radiat. Phys. Chem.* **2001**, 61(1), 19.
- [27] Ö. Şimşek, S. Yilmaz, D. Karagöz, M. Ertugrul, *J. Radioanal. Nucl. Chem.* **2002**, 253(1), 143.
- [28] S. B. Gudennavar, N. M. Badiger, S. R. Thontadarya, B. Hanumaiah, *Radiat. Phys. Chem.* **2003**, 68(5), 721.
- [29] T. Yashoda, S. Krishnaveni, R. Gowda, *Nucl. Instrum. Methods Phys. Res., Sect. B* **2005**, 240(3), 607.
- [30] Y. Ménesguen, M.-C. Lépy, *Nucl. Instrum. Methods Phys. Res., Sect. B* **2010**, 268(16), 2477.
- [31] Ö. Sögüt, *Chin. J. Phys.* **2010**, 48(2), 212.
- [32] W. Bambynek, B. Crasemann, R. W. Fink, H. U. Freund, H. Mark, C. D. Swift, R. E. Price, P. V. Rao, X-ray fluorescence yields, Auger, and Coster-Kronig transition probabilities, **1972**.
- [33] M. O. Krause, *J. Phys. Chem. Ref. Data* **1979**, 8(2), 307.
- [34] Bambynek, X-ray and inner-shell processes in atoms, molecules and solids, **1984**.
- [35] S. Daoudi, A. Kahoul, M. Nekkab, *J. Korean Phys. Soc.* **2015**, 67(9), 1537.

How to cite this article: Martins L, Amaro P, Pessanha S, et al. Multiconfiguration Dirac–Fock calculations of Zn K-shell radiative and nonradiative transitions. *X-Ray Spectrometry*. 2020;49:192–199. <https://doi.org/10.1002/xrs.3089>