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Modified Atomic Orbital Theory Applied to the Study of $(3d^94s\ ^3D_{3,2,1})\boldsymbol{n}$p and the $(3d^94s\ ^1D_2)\boldsymbol{n}$p Rydberg series of Cu-like Zn^+.

Abstract

Precise values of high-lying resonance energies have been determined for the Rydberg series $(3d^94s\ ^3D_{3,2,1})$np and $(3d^94s\ ^1D_2)$np (n ranging from 5 to 45), originating from the ground state $(3d^{10}4s\ ^1S_{1/2})$ of the Cu-like Zn^+ ion. These calculations were carried out within the framework of the Modified Atomic Orbital Theory (MAOT) method.The results show excellent agreement with high-resolution measurements performed at ALS, as well as with calculations obtained using the DARC codes [3] (Dirac Atomic R-matrix Codes) (Hinojoha et al., MNRAS, 470, 4048 (2017)).The analysis is based both on standard quantum defect theory and on the MAOTprocedure, which relies on the calculation of the effective charge. The study highlights the relevance of the MAOT method in complementing experimental data, particularly for the accurate identification of narrow resonance energies affected by overlapping spectral peaks.Finally, new accurate resonance energies for high-lying levels (n = 16 − 45) are proposed as benchmark data to [6] aid in the interpretation of spectra from trans-iron elements in astrophysical environments.

Keywords Photoionization, Resonance Energies, Quantum Defect, Modified Atomic Orbital Theory, Rydberg Series, Synchrotron Radiation

1. Introduction

Resonant photoionization (PI) is a fundamental process in which a photon excites an atom or ion to an unstable intermediate electronic state (autoionizing), which subsequently decays by emitting a free electron. This mechanism leads to a strong enhancement of photoionization cross sections and gives rise to characteristic resonant structures in the spectra. In astrophysical plasmas, such as stellar atmospheres and interstellar media enriched in heavy metals, zinc PI plays a key role in the ionization balance and in determining chemical abundances. Zinc, particularly in the form of Zn II and Zn III ions, is used as an astrophysical tracer since it is only weakly affected by depletion onto interstellar dust. Thus, the study of resonant photoionization of zinc provides constraints on the chemical composition and evolution of stars and galaxies based on UV observations (e.g., with HST and FUSE) (Ferland et al., 1998; Kallman & Palmeri, 2007).

In laboratory plasmas, resonant photoionization of zinc is investigated using synchrotron light sources (ALS, SOLEIL, PETRA III), allowing high-resolution measurements of PI cross sections for different ions (Zn II, Zn III, Zn IV). These experimental measurements provide essential benchmark data to test and validate advanced theoretical models (R-matrix, Dirac Atomic R-matrix Codes – DARC, and semi-empirical methods such as SCUNC) (Peart et al., 1987; Hinojosa et al., 2017; Sakho, 2017, 2018). These studies are also applied to plasma diagnostics and the production of highly charged ions in laboratory physics. Although high-resolution ALS measurements have been conducted and compared with advanced DARC calculations, many spectral peaks of Zn^+ ions remain overlapping, and the corresponding resonances have not been clearly identified. The Modified Atomic Orbital Theory(MAOT) method (Diallo et al. 2018,2025; Sakho, 2011) has proven to be a highly suitable semi-empirical method for accurately reproducing experimental photoionization data. The aim of the present study is to clarify the overlapping ALS lines by using the MAOT method to calculate resonance energies of the $(3d^9\,4s\,D_3)np$, $(3d^9\,4s\,^3D_2)np$, $(3d^9\,4s\,^3D_1)np$, and $(3d^9\,4s\,^1D_2)np$ Rydberg series of Zn^+ ions. Moreover, high-lying Rydberg series provide valuable data for the NIST database, where many resonances are tabulated up to n = 60 for atomic systems such as Mg. This work also aims to extend the ALS measurements (Hinojoh et al., 2017) and associated DARC calculations to higher principal quantum numbers, $n = 16 - 45$. The analysis of the present results is carried out within the framework of standard quantum defect theory and the MAOT procedure, through calculation of the effective charge. The organization of this paper is as follows. Section 2 provides a brief overview of the MAOT formalism, while Section 3 presents the results. The study is concluded in Section 4.

2. Theory

2.1. Brief description of the MAOT formalism

In the framework of the modified atomic orbital theory (MAOT), the total energy of a (νl) given orbital is expressed in the form in Rydberg units (Diallo et al., 2018,2025). □ □ □ □2 2

) ( ) (I I Z I E □ □ □ □ □ □ (1)

The details of this Equation1 are given in our previous papers (Diallo et al., 2025). In the photoionization study, energy resonances En are generally measured relatively to the E∞

converging limit of a given (2S+1LJ)nl- Rydberg series. General expression of the resonance energy En is given by (inRydberg units): 2 1 2 2 1 2 2 1 2 1 2) , , , (1) ( ) ( ) (1) ( ) (1 □ k k J S J S J S n s q m n f q n m n L n L L Z n E E □ □ □ □ (2) In this equation (2), m and q (m□q) denote the principal quantum numbers of the (2S+1LJ)nl Rydberg series of the considered atomic system used in the empirical determination of the) (1 2 J S i L □ □ - screening constants, s represents the spin of the nl-electron (s = 1/2), E□ is the energy value of the series limit generally determined from NIST atomic database, Zrepresents the nuclear charge of the considered element and □ k k s q m n f) , , , (1 is a corrective term introduced to stabilize expression (2). The only problem that one may face by using the MAOT formalism is linked to the determination of the □ □ □ s q m n f , , , -terme. The correct expression of this term is determined iteratively by imposing the general Eq. (2) to provide accurate data with nearly constant or slightly varying quantum defect values along all considered series as the principal quantum number n increases. The value of □is fixed to 1 and or 2 during the iteration.

2.2. Quantum Defect of MOAT

In general, resonance energies are analyzed from the standard quantum-defect expansion formula 2 2) (n core n n RZ E E □ □ □ □

□ (3) In this equation, R=13,60569eVis the Rydberg constant, E∞ denotes the converging limit, Zcorerepresents the electric charge of the core ion, and δ means the quantum defect. From (3), the quantum defect n □ is calculated as follows: □ □ n core n E E R Z n □ □ □ □

□ (4) In addition, introducing the effective nuclear charge Z*, Eq. (2) can be rewritten in the form of Eq. (3) as follows

R n Z E En 22 * □ □ □ (5)

With Z* given by □ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □ k k J S J S J S s q m n f q n m n L n L L Z Z) , , , (1) ( ) ( ) (1) ( ) (1 2 2 1 2 2 1 2 1 * □ □ □ □ (6)

When n tend toward infinity, Eq. (6) tends to the limit □ □ core J S J S core Lim Z Z L L Z Z Z □ □ □ □ □ □ □ □) ( ) (1 2 1 1 2 1 * □ □ (7)

where Zcore is the effective core charge. In the present work, for all the Rydberg series investigated for both Zn II, the resonance energies are given by the formula $En = E\infty - 1\ n2\ Z - \sigma1 - \sigma2 \times 1\ n - \sigma2\ 2 \times n - m \times m - 4s - s2\ n2 \times n + 5m + s\ \ 2\ Ryb$ (8)

3. Results and Discussion

The $\sigma2$ screening constants in Equations (6) and (8) were determined empirically, based on the experimental data reported by Hinojosa et al.(2017). The corresponding values are presented in the table caption. In contrast, the σ_2 screening constant was obtained theoretically from the simple relation $\sigma1 = Z - Zcore$, where the effective core charge ($Zcore$) is directly deduced from the single photoionization process of a given $XP+$ plasma ion. $hv + XP+ \longrightarrow X\ P+1 ++ e- \Longrightarrow Zcore = P + 1$ So, for Cu-like Zn II ion, we find. $hv + Zn+ \longrightarrow Zn2++ e-;\ Zcore = 2 \Longrightarrow \sigma1 = 28$ The resonance energies of the I ($3d^9 4s\ ^3D_3$)np, II ($3d^9 4s\ ^3D_2$)np, III ($3d^9 4s\ ^3D_1$) np, IV ($3d^9 4s\ ^1D_2$) np, and V ($3d^9 4s\ ^3D_3$)np Rydberg series, originating from the ($3d^{10} 4s$) $^1S1/2$ ground state of Zn^+ ions, are reported in Tables 1–5. The present MAOT calculations are compared with results obtained using the SCUNC method (Badiane et al., 2019) as well as with ALS experimental data (Hinojoha et al., 2017). In the ALS studies, resonance energies were determined only up to $n = 15$ (see Table 4). Generally, because of configuration interaction and electron–electron correlation effects, cross-section peaks tend to overlap, making the identification of spectral lines increasingly difficult as n increases. Nevertheless, the MAOT approach proves sufficiently stable to tabulate very high-lying resonances up to

n = 45, with the quantum defect remaining nearly constant across all the series investigated. Furthermore, for several resonances, uncertain experimental entries indicated in parentheses are clarified. Table 1 presents the quantum defects and resonance energies of the $(3d^94s\ ^3D_3)np$ Rydberg series, originating from the $3d^{10}4s\ ^1S1/2$ ground state of Zn^+ and converging to the $(3d^94s\ ^3D_3)$ series limit of Zn^{2+}. Four uncertain ALS values are reported for the 7p, 9p, 11p, and 12p levels at [26.093 eV], [26.773 eV], [27.087 eV], and [27.184 eV], respectively. These are compared with the present MAOT predictions of 26.097 eV, 26.778 eV, 27.092 eV, and 27.189 eV, and with the SCUNC results of Badiane et al. (2019), which give 26.102 eV, 26.782 eV, 27.095 eV, and 27.192 eV. The maximum discrepancy between ALS data and the new MAOT calculations is 0.005 eV, while it rises to 0.009 eV in the values of Badiane et al. (2019). For n = 6 and 8, the MAOT energies (25.409 eV and 26.510 eV) show excellent agreement with ALS measurements (25.408 eV and 26.512 eV; Hinojoha et al., 2017). Across all resonances, the MAOT quantum defect remains nearly constant, ranging from 1.1 to 1.2, consistent with the ALS average value of 1.11 ± 0.2 (Hinojoha et al., 2017).Tables 2 and 3lists resonance energies and quantum defects of the Rydberg series $(3d^94s\ ^3D_2)np$ and $(3d^94s\ ^3D_1)np$, originating from the ground state $(3d^{10}4s)\ ^1S1/2$ of Zn^+ ions and converging respectively to the $(3d^94s\ ^3D_2)$ and $(3d^94s\ ^3D_1)$ series limits of Zn^{2+}. The results obtained with the MAOT method are compared with ALS experimental measurements (Hinojoha et al., 2017) as well as with the SCUNC predictions (Badiane et al., 2019).For the $(3d^94s\ ^3D_2)np$ and $(3d^94s\ ^3D_1)np$ series, uncertain ALS values were identified at the 10p and 9p states, with corresponding energies of [27.104 eV] and [27.116 eV]. The MAOT predictions for these states are 27.108 eV and 27.121 eV, yielding deviations of only 0.004 eV and 0.005 eV, respectively, from the ALS data. For the remaining resonances between n = 5 and n = 10, the agreement between theory and experiment is excellent, with energy differences never exceeding 0.008 eV.Moreover, the quantum defect predicted by MAOT remains nearly constant, ranging between 1.1 and 1.2. Finally, for the two

($3d^9 4s\ ^3D$)np Rydberg series originating from the ground state ($3d^{10}4s\ ^1S_1/_2$) of Zn^+, the MAOT results are extended up to n = 45, confirming an almost invariant quantum defect throughout the series.In the Table 4 we havethe resonance energies and quantum defect of the ($3d^9 4s\ ^1D_2$)np Rydberg series, originating from the ($3d^{10}4s\ ^1S1/2$) ground state of the Zn^+ ion and converging to the ($3d4s\ ^1D_2$) series limit of Zn^{2+}. The results obtained using the MAOT method are compared with ALS experimental data (Hinojoha et al., 2017) as well as with the theoretical predictions of the SCUNC model (Badiane et al., 2019).Three

characteristic resonances($3d^9 4s\ ^1D_2$)6p, ($3d^9 4s\ ^1D_2$)7p, and ($3d^9 4s\ ^1D_2$)8pare identified as overlapping states. Their resonance energies, 26.080 eV, 26.769 eV, and 27.183 eV, respectively, are in close agreement with both the MAOT predictions (26.081 eV, 26.770 eV, and 27.184 eV) and those from the SCUNC model. For the ($3d^9 4s\ ^1D_2$)8p state, the MAOT value shows particularly good agreement with experiment, with a deviation of only 0.001 eV, compared to 0.006 eV for the SCUNC prediction, confirming the reliability of this result.Except for the ($3d^9 4s\ ^1D_2$)6p state, which shows a shift of 0.011 eV, the maximum discrepancy between the new calculations and the experimental data remains below 0.07 eV. For levels n = 9 to 15, the agreement between MAOT values and ALS measurements is excellent, with differences never exceeding 0.006 eV. Finally, the quantum defect of this Rydberg series remains nearly constant, between 1.1 and 1.2.TheTable 5 shows the resonance energies and quantum defects of the ($3d^9 4s\ ^3D_3$)np Rydberg series, originating from the ($3d^{10}4s\ ^1S1/2$) ground state of the Zn^+ ion and converging to the ($3d^9 4s\ ^3D_3$) series limit of Zn^{2+}. The results obtained using the MAOT method are compared with the experimental ALS measurements (Hinojoha et al., 2017). For this series, two overlapping resonances were identified, corresponding to the 8p and 9p states, located at 26.340 eV and 26.714 eV, respectively. The MAOT predictions for these levels are 26.404 eV and 26.711 eV, yielding a maximum energy difference of 0.064 eV.It is worth noting that the SCUNC method (Badiane et al., 2019) encountered difficulties in providing reliable data for this series, highlighting the relevance of the MAOT predictions as a reference for future high-resolution measurements. Finally, for all resonances considered, the quantum defect remains nearly constant, within the range 1.4-1.5.Tables 6 and 7compare resonance energies of the (3d^{9}4s $^3D_3$)np and (3d^{9}4s $^3D_2$)np series, as well as the (3d^{9}4s $^3D_1$)np and (3d^{9}4s $^1D_2$)np series, all originating from the 3d^{10}4s $^1S1/2$ ground state of Zn^+ and converging respectively to the (3d^{9}4s $^3D_3$) and (3d^{9}4s $^3D_2$) limits of Zn^{2+}. [2] The present MAOT results are compared with ALS measurements, the Dirac Coulomb R-matrix (DARC) calculations of Hinojoha et al. (2017), and the pioneering merged-beams experiments of Peart et al. (1987) conducted at the Daresbury synchrotron facility. The comparison indicates that MAOT predictions agree more closely with ALS data than other theoretical approaches. The maximum relative deviation is only 0.04% for the (3d^{9}4s $^3D_3$)7p state, mainly due to experimental uncertainties in the ALS value [26.093 eV]. In contrast, the DARC method shows a deviation of 0.07% for the same state, while the DAR approach exhibits a larger deviation of 0.24% at the (3d^{9}4s $^3D_2$)7p level.

Tableau 1:Resonance energies (E) and quantum defect (δ) of the (3d94s 3D3)np Rydberg series I originate from the (3d104s) 1S1/2 ground state of the Zn+ ions converging to the (3d94s 3D3) series limit of Zn2+. [2] The present MAOT results are compared with the SCUNC results (Badiane et al., 2017) and the ALS experimental data (Hinojoha et al., 2017). The ALS energies are calibrated to ± 0,017 eV.σ1(2D5/2) = −0.770 ± 0.048; σ2(2D5/2) = 28.00. n I(3d94s3D3)np MAOT SCUNC ALS MAOT SCUNC □ E E E |ΔE| |ΔE| 5 1,1 24,141 24,141 24,141 0.000 0.000 6 1,1 25,409 25,415 25,408 0.001 0.007 7 1,1 26,097 26,102 [26,093] [0.004] [0.009] 8 1,1 26,510 26,515 26,512 0.002 0.003 9 1,1 26,778 26,782 [26,773] [0.005] [0.009] 10 1,1 26,961 26,965 26,966 0.005 0.001 11 1,1 27,092 27,096 [27,087] 0.005 [0.008] 12 1,1 27,189 27,192 [27,184] 0.005 [0.008] 13 1,1 27,262 27,265 (27,253) (0.009) (0.012) 14 1,1 27,320

27,321 15 1,1 27,365 27,367 16 1,1 27,401 27,403 17 1,1 27,431 27,433 18 1,1 27,456 27,457 19 1,1 27,477 27,478 20 1,1 27,494 27,495 21 1,1 27,509 27,510 22 1,1 27,522 27,523 23 1,1 27,533 27,534 24 1,1 27,543 27,543 25 1,1 27,551 27,552 26 1,2 27,559 27,559 27 1,2 27,566 27,566 28 1,2 27,571 27,572 29 1,2 27,577 27,577 30 1,2 27,582 27,582 31 1,2 27,586 27,586 32 1,2 27,590 27,590 33 1,2 27,593 27,594 34 1,2 27,596 27,597 35 1,2 27,599 27,600 36 1,2 27,602 27,602 37 1,2 27,605 27,605 38 1,2 27,607 27,607 39 1,2 27,609 27,609 40 1,2 27,611 27,611 41 1,2 27,613 - 42 1,2 27,614 - 43 1,2 27,616 - 44 1,2 27,617 - 45 1,2 27,619 -

Tableau 2:Resonance energies (E) and quantum defect (δ) of the (3d94s 3D2)np Rydberg 188 series II originate from the (3d104s) 1S1/2 ground state of the Zn+ ions converging to the (3d94s 189 3D2) series limit of Zn2+. The present MAOT results are compared with the SCUNC results 190 (Badiane et al., 2017) and the ALS experimental data (Hinojoha et al., 2017). The ALS 191 energies are calibrated to ± 0,017 eV. 192 n II(3d94s3D2)np MAOT SCUNC ALS MAOT SCUNC □ E E E |ΔE| |ΔE| 5 1,1 24,294 24,294 24,294 0.000 0.000 6 1,1 25,559 25,564 25,569 0.010 0.005 7 1,1 26,245 26,250 26,243 0.002 0.007 8 1,1 26,658 26,662 26,656 0.002 0.006 9 1,1 26,925 26,929 26,926 0.001 0.003 10 1,1 27,108 27,112 [27,104] [0.004] [0.008] 11 1,1 27,239 27,242 12 1,1 27,335 27,338 13 1,1 27,409 27,411 14 1,1 27,466 27,468 15 1,1 27,511 27,513 16 1,1 27,547 27,549 17 1,1 27,577 27,579 18 1,1 27,602 27,603 19 1,1 27,623 27,623 20 1,1 27,640 27,641 21 1,1 27,655 27,656 22 1,1 27,668 27,669 23 1,1 27,679 27,680 24 1,1 27,689 27,690 25 1,1 27,697 27,698 26 1,2 27,705 27,705 27 1,2 27,712 27,712 28 1,2 27,717 27,718 29 1,2 27,723 27,723 30 1,2 27,728 27,728 31 1,2 27,732 27,732 32 1,2 27,736 27,736 33 1,2 27,739 27,740 34 1,2 27,743 27,743 35 1,2 27,745 27,746 36 1,2 27,748 27,748 37 1,2 27,751 27,751 38 1,2 27,753 27,753 39 1,2 27,755 27,755 40 1,2 27,757 27,757 41 1,2 27,759 - 42 1,2 27,760 - 43 1,2 27,762 - 44 1,2 27,763 - 45 1,2 27,765 -

Tableau 3:Resonance energies (E) and quantum defect (δ) of the (3d94s 3D1)np Rydberg 193 series III originate from the (3d104s) 1S1/2 ground state of the Zn+ ions converging to the 194 (3d94s 3D1) series limit of Zn2+. 2 The present MAOT results are compared with the SCUNC 195 results (Badiane et al., 2017) and the ALS experimental data (Hinojoha et al., 2017). The ALS 196 energies are calibrated to ± 0,017 eV. 197 n III(3d94s3D1)np MAOT SCUNC ALS MAOT SCUNC E E E |ΔE| |ΔE| 5 1,1 24,488 24,488 24,488 0.000 0.000 6 1,1 25,754 25,759 25,752 0.002 0.007 7 1,1 26,440 26,446 26,439 0.001 0.007 8 1,1 26,853 26,858 26,858 0.005 0.000 9 1,1 27,121 27,125 [27,116] [0.005] [0.009] 10 1,1 27,304 27,307 11 1,1 27,435 27,438 12 1,1 27,531 27,534 13 1,1 27,605 27,607 14 1,1 27,662 27,664 15 1,1 27,707 27,709 16 1,1 27,743 27,745 17 1,1 27,773 27,775 18 1,1 27,798 27,799 19 1,1 27,819 27,820 20 1,1 27,836 27,837 21 1,1 27,851 27,852 22 1,1 27,864 27,865 23 1,1 27,875 27,876 24 1,1 27,885 27,885 25 1,1 27,893 27,894 26 1,2 27,901 27,901 27 1,2 27,908 27,908 28 1,2 27,913 27,914 29 1,2 27,919 27,919 30 1,2 27,924 27,924 31 1,2 27,928 27,928 32 1,2 27,932 27,932 33 1,2 27,935 27,936 34 1,2 27,939 27,939 35 1,2 27,941 27,942 36 1,2 27,944 27,944 37 1,2 27,947 27,947 38 1,2 27,949 27,949 39 1,2 27,951 27,951 40 1,2 27,953 27,953 41 1,2 27,955 - 42 1,2 27,956 - 43 1,2 27,958 - 44 1,2 27,959 - 45 1,2 27,961 -

Tableau 4:Resonance energies (E) and quantum defect (δ) of the (3d94s 1D2)np Rydberg 198 series IV originate from the (3d104s) 1S1/2 ground state of the Zn+ ions converging to the 199 (3d94s 1D2) series limit of Zn2+. 2 The present MAOT results are compared with the SCUNC 200 results (Badiane et al., 2017) and the ALS experimental data (Hinojoha et al., 2017). The ALS 201 energies are calibrated to ± 0,017 eV. 202 n IV(3d94s1D2)np MAOT SCUNC ALS MAOT SCUNC E E E |ΔE| |ΔE| 5 1,1 24,804 24,804 24,804 0.000 0.000 6 1,1 26,080 26,081 [26,069] [0.011] [0.012] 7 1,1 26,769 26,770 [26,773] [0.004] [0.003] 8 1,1 27,183 27,178 [27,184] [0.001] [0.006] 9 1,1 27,450

27,451 27,450 0.000 0.001 10 1,1 27,633 27,634 27,632 0.001 0.002 11 1,1 27,764 27,765 27,767 0.003 0.002 12 1,1 27,860 27,861 27,863 0.003 0.002 13 1,1 27,933 27,934 27,939 0.006 0.005 14 1,1 27,990 27,991 27,994 0.004 0.003 15 1,1 28,035 28,036 28,041 0.006 0.005 16 1,1 28,072 28,072 17 1,1 28,102 28,102 18 1,1 28,126 28,126 19 1,1 28,147 28,147 20 1,1 28,164 28,164 21 1,1 28,179 28,179 22 1,1 28,192 28,192 23 1,1 28,203 28,203 24 1,1 28,213 28,213 25 1,1 28,221 28,221 26 1,2 28,229 28,229 27 1,2 28,236 28,236 28 1,2 28,242 28,242 29 1,2 28,247 28,247 30 1,2 28,252 28,252 31 1,2 28,256 28,256 32 1,2 28,260 28,260 33 1,2 28,263 28,263 34 1,2 28,267 28,267 35 1,2 28,269 28,269 36 1,2 28,272 28,272 37 1,2 28,275 28,275 38 1,2 28,277 28,277 39 1,2 28,279 28,279 40 1,2 28,281 28,281 41 1,2 28,283 - 42 1,2 28,284 - 43 1,2 28,286 - 44 1,2 28,287 - 45 1,2 28,289 -

Tableau 5:Resonance energies (E) and quantum defect (δ) of the (3d94s 3D3)np Rydberg 203 series V originate from the (3d104s) 1S1/2 ground state of the Zn+ ions converging to the (3d94s 204 3D3)series limit of Zn2+. The present MAOT results are compared with the SCUNC results 205 (Badiane et al., 2017) and the ALS experimental data (Hinojoha et al., 2017). The ALS 206 energies are calibrated to ± 0,017 eV. 207 n V(3d94s3D3)np MAOT ALS |ΔE| □ E E 6 1,4 25,071 25,071 0,000 7 1,4 25,917 25,910 0,007 8 1,4 26,404 (26,340) (0,064) 9 1,4 26,711 (26,714) (0,003) 10 1,4 26,916 11 1,4 27,061 12 1,4 27,166 13 1,4 27,245 14 1,4 27,306 15 1,4 27,354 16 1,4 27,393 17 1,4 27,424 18 1,4 27,450 19 1,4 27,472 20 1,4 27,490 21 1,4 27,505 22 1,4 27,519 23 1,4 27,530 24 1,5 27,540 25 1,5 27,549 26 1,5 27,557 27 1,5 27,564 28 1,5 27,570 29 1,5 27,575 30 1,5 27,580 31 1,5 27,585 32 1,5 27,589 33 1,5 27,592 34 1,5 27,596 35 1,5 27,599 36 1,5 27,601 37 1,5 27,604 38 1,5 27,606 39 1,5 27,608 40 1,5 27,610 41 1,5 27,612 42 1,5 27,614 43 1,5 27,615 44 1,5 27,617 45 1,5 27,618 208

Tableau 6: Comparison of resonance energies of the (3d94s 3D3)np and (3d94s 3D2)np

Rydberg series originating from the (3d104s) 1S1/2 ground state of the Zn+ ions converging to the (3d94s 3D3) and (3d94s 3D2) series limits respectively of Zn2+. n (3d94s3D3)np Rydberg series (3d94s3D2)np Rydberg series MAOT E DARC E ALS E DAR E MAOT E DARC E ALS E DAR E 5 24,141 24,158 24,141 24,172 24,294 24,312 24,294 24,329 6 25,409 25,418 25,408 25,468 25,559 25,577 25,569 25,616 7 26,097 26,102 [26,093] 26,150 26,245 26,251 26,243 26,305 8 26,510 26,512 26,658 26,656 9 26,778 [26,773] 26,925 26,926 10 26,961 26,966 27,108 [27,104] 11 27,092 [27,087] 27,239 12 27,189 [27,184] 27,335 13 27,262 (27,253) 27,409 MAOT, Modified Atomic Orbital Theory , present calculations. DARC, Dirac Atomic R-matrix Codes, (Hinojoha et al., 2017). ALS, experimental results, (Hinojoha et al., 2017). DAR, DARESBURY, experimental results (Peart et al., 1987). Tableau 7: Comparison of resonance energies of the (3d94s 3D1)np and (3d94s 1D2)np Rydberg series originating from the (3d104s) 1S1/2 ground state of the Zn+ ions converging to the (3d94s 3D1) and (3d94s 1D2) series limits respectively of Zn2+. n (3d94s 3D1)np Rydberg series (3d94s 1D2)np Rydberg series MAOT E DARC E ALS E DAR E MAOT E DARC E ALS E DAR E 5 24,488 24,504 24,488 24,509 24,804 24,824 24,804 24,839 6 25,754 25,762 25,752 25,786 26,080 [26,069] 7 26,440 26,439 26,769 [26,773] 8 26,853 26,858 27,183 [27,184] 9 27,121 [27,116] 27,450 27,450 10 27,304 27,633 27,632 11 27,435 27,764 27,767 12 27,531 27,860 27,863 13 27,605 27,933 27,939 14 27,662 27,990 27,994 15 27,707 28,035 28,041 MAOT, Modified Atomic Orbital Theory , present calculations. DARC, Dirac Atomic R-matrix Codes, (Hinojoha et al., 2017). ALS, experimentalresults, (Hinojoha et al., 2017). DAR, DARESBURY, experimentalresults (Peart et al., 1987).

4. Conclusion The Modified Atomic Orbital Theory (MAOT)formalism has been applied to the photoionization study of the $(3d^94s\ ^3D_{3,\ 2,\ 1})n$p and $(3d^94s\ ^1D_2)n$p (n = 5

− 45)Rydberg series, originating from the ($3d^{10}4s$ $^{1}S1/2$) ground state of the Zn^{+} ion. Overall, the results obtained show excellent agreement with high-resolution ALS measurements, as well as with Dirac–Coulomb R-matrix calculations [(Hinojoha et al., 2017), MNRAS, 000, 1] and theoretical predictions from the SCUNC method (Badiane et al., 2019). This work demonstrates the ability of the MAOT approach to support experiments in resolving very closely spaced resonance energies, particularly in the presence of overlapping peaks. The newly determined resonance energies, obtained with high precision, are proposed as reference data for the interpretation of Zn^{+} spectra observed in nebulae. Furthermore, these high-lying Rydberg series provide a valuable contribution to the enrichment of the NIST atomic database.

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DATA AVAILABILITY

All data generated or analyzed during this study are included in this published article.

CONFLICT OF INTEREST

The authors of this work declare that they have no conflicts of interest

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