Modified Atomic Orbital Theory Applied to the Study of $(3d^9 4s\ ^3D_{3,2,1})np$ and the $(3d^9 4s\ ^1D_2)np$ Rydberg series of Cu-like Zn^+.

Abstract

Precise values of high-lying resonance energies have been determined for the Rydberg series $(3d^9 4s\ ^3D_{3,2,1})np$ and $(3d^9 4s\ ^1D_2)np$ (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 (*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 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 (vl)-given orbital is expressed in the form in Rydberg units (Diallo et al., 2018,2025).

$$E(vl) = -\frac{[Z - \sigma(l)]^2}{v(l)^2} \qquad (1)$$

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 $E\infty$

converging limit of a given ($^{2S+1}L_J$)*nl*- Rydberg series. General expression of the resonance energy *En* is given by (inRydberg units):

$$E_n = E_\infty - \frac{1}{n^2}\left\{Z - \sigma_1(^{2S+1}L_J) - \sigma_2(^{2S+1}L_J)\times\frac{1}{n} - \sigma_2^{\alpha}(^{2S+1}L_J)\times(n-m)\times(n-q)\sum_k \frac{1}{f_k(n,m,q,s)}\right\}^2 \quad (2)$$

In this equation (2), *m* and *q* (*m*<*q*) denote the principal quantum numbers of the ($^{2S+1}L_J$)*nl*-Rydberg series of the considered atomic system used in the empirical determination of the $\sigma_i(^{2S+1}L_J)$ - 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, *Z*represents the nuclear charge of the considered element and $\sum_k \frac{1}{f_k(n,m,q,s)}$ 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 $\sum f(n,m,q,s)$-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 $\alpha$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

$$E_n = E_\infty - \frac{RZ_{core}^{\ 2}}{(n-\delta_n)^2} \quad (3)$$

In this equation, *R*=13,60569eVis the Rydberg constant, *E*∞ denotes the converging limit, Z_{core}represents the electric charge of the core ion, and $\boldsymbol{\delta}$ means the quantum defect.

From (3), the quantum defect δ_n is calculated as follows:

$$\delta_n = n - Z_{core}\sqrt{\frac{R}{(E_\infty - E_n)}}$$

(4)

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

$$E_n = E_\infty - \frac{Z^{*2}}{n^2} R \quad (5)$$

With Z* given by

$$Z^* = \left\{ Z - \sigma_1(^{2S+1}L_J) - \sigma_2(^{2S+1}L_J) \times \frac{1}{n} - \sigma_2^{\alpha}(^{2S+1}L_J) \times (n-m) \times (n-q) \sum_k \frac{1}{f_k(n,m,q,s)} \right\}$$

(6)

When *n* tend toward infinity, Eq. (6) tends to the limit

$$Z^*_{Lim} = Z_{core} = \left\{ Z - \sigma_1(^{2S+1}L_J) \right\} \Rightarrow \sigma_1(^{2S+1}L_J) = Z - Z_{core}$$

(7)

where Z_{core} 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

$$E_n = E_\infty - \frac{1}{n^2} \left\{ Z - \sigma_1 - \sigma_2 \times \frac{1}{n} - \sigma_2^2 \times \frac{(n-m) \times (m - 4s - s^2)}{n^2 \times (n + 5m + s)} \right\}^2 Ryb \quad (8)$$

3. Results and Discussion

The σ_2 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 σ₂ screening constant was obtained theoretically from the simple relation $\sigma_1 = Z - Z_{core}$, where the effective core charge (Z_{core}) is directly deduced from the single photoionization process of a given X^{P+} plasma ion.

$$h\upsilon + X^{P+} \longrightarrow X^{(P+1)+} + e^- \Longrightarrow Z_{core} = (P+1)$$

So, for Cu-like Zn II ion, we find.

$$h\upsilon + Zn^{+} \longrightarrow Zn^{2+} + e^-;\ Z_{core} = 2 \Longrightarrow \sigma_1 = 28$$

The resonance energies of the I ($3d^9 4s\ ^3D_3$)*n*p, II ($3d^9 4s\ ^3D_2$)*n*p, III ($3d^9 4s\ ^3D_1$) *n*p, IV ($3d^9 4s\ ^1D_2$) np, and V ($3d^9 4s\ ^3D_3$)*n*p Rydberg series, originating from the ($3d^{10} 4s$) $^1S_{1/2}$ 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 ($3d^9 4s\ ^3D_3$)np Rydberg series, originating from the $3d^{10}4s\ ^1S_{1/2}$ ground state of Zn^+ and converging to the ($3d^9 4s\ ^3D_3$) 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 3**lists resonance energies and quantum defects of the Rydberg series ($3d^9 4s\ ^3D_2$)np and ($3d^9 4s\ ^3D_1$)np, originating from the ground state ($3d^{10}4s$) $^1S_{1/2}$ of Zn^+ ions and converging respectively to the ($3d^9 4s\ ^3D_2$) and ($3d^9 4s\ ^3D_1$) 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 ($3d^9 4s\ ^3D_2$)np and ($3d^9 4s\ ^3D_1$)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 ($3d^{10}4s\ ^1S_{1/2}$) 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.The**Table 5** shows the resonance energies and quantum defects of the ($3d^9 4s\ ^3D_3$)np Rydberg series, originating from the ($3d^{10} 4s\ ^1S_{1/2}$) 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 7**compare 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 $3d^{10} 4s\ ^1S_{1/2}$ ground state of Zn^+ and converging respectively to the ($3d^9 4s\ ^3D_3$) and ($3d^9 4s\ ^3D_2$) limits of Zn^{2+}. 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 ($3d^9 4s\ ^3D_3$)np Rydberg series I originate from the ($3d^{10}4s$) $^1S_{1/2}$ ground state of the Zn^+ ions converging to the ($3d^9 4s\ ^3D_3$) series limit of Zn^{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.

		I($3d^9 4s^3D_3$)np				
		MAOT	SCUNC	ALS	MAOT	SCUNC
n	δ	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 ($3d^9 4s\ ^3D_2$)np Rydberg series II originate from the ($3d^{10}4s$) $^1S_{1/2}$ ground state of the Zn^+ ions converging to the ($3d^9 4s\ ^3D_2$) series limit of Zn^{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.

		II($3d^9 4s^3D_2$)np				
		MAOT	SCUNC	ALS	MAOT	SCUNC
n	δ	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 ($3d^9 4s\ ^3D_1$)np Rydberg series III originate from the ($3d^{10}4s$) $^1S_{1/2}$ ground state of the Zn^+ ions converging to the ($3d^9 4s\ ^3D_1$) series limit of Zn^{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.

		III($3d^9 4s^3D_1$)np				
		MAOT	SCUNC	ALS	MAOT	SCUNC
n	δ	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 ($3d^9 4s\ ^1D_2$)np Rydberg series IV originate from the ($3d^{10}4s$) $^1S_{1/2}$ ground state of the Zn^+ ions converging to the ($3d^9 4s\ ^1D_2$) series limit of Zn^{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.

		IV($3d^9 4s\ ^1D_2$)np				
		MAOT	SCUNC	ALS	MAOT	SCUNC
n	δ	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 ($3d^9 4s\ ^3D_3$)np Rydberg series V originate from the ($3d^{10}4s$) $^1S_{1/2}$ ground state of the Zn^+ ions converging to the ($3d^9 4s\ ^3D_3$)series limit of Zn^{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.

		V($3d^9 4s^3D_3$)np		
		MAOT	ALS	
n	δ	E	E	|ΔE|
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		

Tableau 6: Comparison of resonance energies of the ($3d^9 4s\ ^3D_3$)np and ($3d^9 4s\ ^3D_2$)np Rydberg series originating from the ($3d^{10} 4s$) $^1S_{1/2}$ ground state of the Zn^+ ions converging to the ($3d^9 4s\ ^3D_3$) and ($3d^9 4s\ ^3D_2$) series limits respectively of Zn^{2+}.

n	($3d^9 4s^3D_3$)np Rydberg series				($3d^9 4s^3D_2$)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 ($3d^9 4s\ ^3D_1$)np and ($3d^9 4s\ ^1D_2$)np Rydberg series originating from the ($3d^{10} 4s$) $^1S_{1/2}$ ground state of the Zn^+ ions converging to the ($3d^9 4s\ ^3D_1$) and ($3d^9 4s\ ^1D_2$) series limits respectively of Zn^{2+}.

n	($3d^9 4s\ ^3D_1$)np Rydberg series				($3d^9 4s\ ^1D_2$)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 ($3d^9 4s\ ^3D_{3,\ 2,\ 1}$)np and ($3d^9 4s\ ^1D_2$)np ($n = 5 - 45$)Rydberg series, originating from the ($3d^{10} 4s\ ^1S_{1/2}$) 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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