

Photoionization Study of the $4s^24p^4(^3P_1)nd$, $4s^24p^4(^1D_2)nd$ and $4s^24p^4(^1S_0)nd$ Rydberg Series of Rb^{2+} via the Modified Atomic Orbital Theory

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Abstract

We consider the $4s^24p^4(^3P_1)nd$, $4s^24p^4(^1D_2)nd$ and $4s^24p^4(^1S_0)nd$ Rydberg series of Rb^{2+} originating from the $4s^24p^5(^2P_{1/2})$ ground state and $4s^24p^5(^2P_{3/2})$ metastable state of Rb^{2+} converging respectively to the $4s^24p^4(^3P_1)$, $4s^24p^4(^1D_2)$ and $4s^24p^4(^1S_0)$ series limit in Rb^{3+} . The semi-empirical procedure of Modified Atomic Orbital Theory (MAOT) is applied to perform calculations in the present work from $n = 6$ up to $n = 45$. We note that the MAOT procedure gives accurate results compared to available Advanced Light Source (ALS) experimental data and other theoretical results. We tabulate new data from $n = 22 - 45$ for $4s^24p^4(^1S_0)nd$ Rydberg series originating from the $4s^24p^5(^2P_{1/2})$ ground state and $4s^24p^5(^2P_{3/2})$ metastable state of Rb^{2+} . The other Rydberg series $4s^24p^4(^3P_1)nd$ and $4s^24p^4(^1D_2)nd$ are extended up to $n = 45$.

Keywords

Rydberg Series, MAOT, Photoionization, Ground State, Metastable State, Atomic Ions, Semi-Empirical Procedure

1. Introduction

Photoionization of atomic ions is a fundamental process that occurs in the astrophysical environments like stars and nebulae [1] [2] where the temperature is suf-

efficient to ionize the matter. Most of the chemical heavier elements than iron are produced by slow neutron capture process or rapid neutron capture process and the Rubidium (Rb) is one of these elements [3] [4]. The provision of data obtained from the photoionization of Rubidium is a valuable aid to the simulation of astrophysical phenomena involving this element, particularly in the nucleosynthesis of heavy elements. Macaluso *et al.* [5] used a third-generation synchrotron radiation and the photo-ion, merged-beams technique at Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory with a band pass resolution of 13.5 ± 2.5 meV full width half maximum (FWHM) to perform high-resolution photoionization cross section measurements of the for Rb^{2+} over the photon energy range 37.31 - 44.08 eV spanning the $4s^2 4p^5(^2P_{3/2})$ ground state and $4s^2 4p^5(^2P_{1/2})$ metastable state ionization thresholds. They identify three distinct Rydberg resonance series $4s^2 4p^4(^3P_1)nd$, $4s^2 4p^4(^1D_2)nd$ and $4s^2 4p^4(^1S_0)nd$ originating from the $4s^2 4p^5(^2P_{3/2})$ ground state and $4s^2 4p^5(^2P_{1/2})$ metastable state. In tandem with the measurements, Breit-Pauli R-matrix calculations were performed in the intermediate coupling jK to facilitate the identification of several highly excited Auger Rydberg resonance states of the Rb^{2+} ions. Using a fully relativistic approach within the Dirac-Coulomb R-Matrix approximation (DARC), McLaughlin *et al.* [6] calculated the cross sections for the $4s^2 4p^5(^2P_{3/2})$ ground state and the corresponding $4s^2 4p^5(^2P_{1/2})$ metastable state. They used the high-resolution ALS photoionization cross sections to benchmark their PI cross sections and Auger Rydberg resonances. They obtained excellent results providing confidence in the theoretical data for astrophysical applications. Employing the Screen Constant by Unit Nuclear Charge (SCUNC), Sakho *et al.* [7] determined the energy resonances of the $4s^2 4p^4(^3P_1)nd$ and $4s^2 4p^4(^1D_2)nd$ Rydberg series until $n = 40$ and reported precise high lying photoionization data of Rb^{2+} ions reducing energy deviations with respect to ALS data at a maximum of 0.001 eV. The Modified Atomic Orbital Theory (MAOT) has been applied successfully in the studies of trans-iron Photoionization by Diop *et al.* [8]. In this paper, we apply the MAOT formalism to investigate the $4s^2 4p^4(^3P_1)nd$, $4s^2 4p^4(^1D_2)nd$ and $4s^2 4p^4(^1S_0)nd$ prominent Rydberg series in the photoionization spectra of Rb^{2+} .

In **Section 2**, we present the theoretical procedure adopted in this work with a brief description of the MAOT formalism and the analytical expressions used in the calculations.

In **Section 3**, we present and discuss the results obtained along. The present results are compared with experimental data of Macaluso *et al.* [5] [9], the Dirac-Coulomb R-Matrix approximation (DARC) calculations of McLaughlin *et al.* [6] and SCUNC calculations of Sakho *et al.* [7].

In **Section 4**, we summarize and conclude the present work.

2. Theory

2.1. Brief Description of the MOAT Formalism

In the framework of Modified Atomic Orbital Theory (MAOT), total energy of (ν)-

given orbital is expressed in the form [10]-[13]

$$E = -\frac{[Z - \sigma_i(l)]^2}{v_i^2} \quad (1)$$

For an atomic system of several electrons M, the total energy is given by (in Rydberg):

$$E = -\sum_{i=1}^N \frac{[Z - \sigma_i(l)]^2}{v_i^2}$$

With respect to the usual spectroscopic notation $(Nl, n'l')^{2S+1}L^{\pi}$, this equation becomes

$$E = -\sum_{i=1}^N \frac{[Z - \sigma_i(2S+1L^{\pi})]^2}{v_i^2} \quad (2)$$

In the photoionization of atoms and ions, energy resonances are generally measured relatively to the E_{∞} converging limit of a given $(2S+1L_J)nl$ -Rydberg series. For these states, the general expression of the energy resonances E_n is given by the formula of Sakho presented previously [8] (in Rydberg units)

$$E = E_{\infty} - \frac{1}{n^2} \left[Z - \sigma_1(2S+1L_J) - \sigma_2(2S+1L_J) \times \frac{1}{n} - \sigma_2^{\alpha}(2S+1L_J) \times (n-m) \times (n-q) \sum_k \frac{1}{f_k(n, m, q, s)} \right]^2 \quad (3)$$

In this equation, m and q ($m < q$) denote the principal quantum numbers of the $(2S+1L_J)nl$ -Rydberg series of the considered atomic system used in the empirical determination of the $\sigma_i(2S+1L_J)$ -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, E_n denotes the corresponding energy resonance, and Z represents the nuclear charge of the considered element.

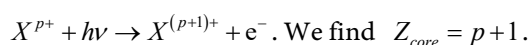
The only problem that one may face by using the MAOT formalism is linked to the determination of the $\sum_k \frac{1}{f_k(n, m, q, s)}$ term.

The correct expression of this term is determined iteratively by imposing general Equation (3) to give accurate data with a constant quantum defect values along all the considered series. The value of α is generally fixed to 1 and or 2 during the iteration. The quantum defect (δ) is calculated from the standard formula below:

$$E_n = E_{\infty} - \frac{RZ_{core}^2}{(n-\delta)^2} \Rightarrow \delta = n - Z_{core} \sqrt{\frac{R}{E_{\infty} - E_n}} \quad (4)$$

In this equation, R is the Rydberg constant, E_{∞} is the converging limit, Z_{core} represents the electric charge of the core ion, and δ is the quantum defect.

Z_{core} is directly obtained by the photoionization process from an atomic X^{p+} system:



In addition, theoretical and measured energy positions can be analyzed by calculating the Z effective charge in relationship with the quantum defect (δ).

The relationship between Z^* and δ is in this form below:

$$Z^* = \frac{Z_{core}}{1 - \frac{\delta}{n}} \tag{5}$$

According to this equation, each Rydberg series must satisfy the following conditions:

$$\begin{cases} Z^* \geq Z_{core} & \text{if } \delta \geq 0 \\ Z^* < Z_{core} & \text{if } \delta < 0 \\ \lim_{n \rightarrow \infty} Z^* = Z_{core} \end{cases} \tag{6}$$

2.2. Energy Resonances of the $4s^2 4p^4(^3P_1)nd$, $4s^2 4p^4(^1D_2)nd$ and $4s^2 4p^4(^1S_0)nd$ Rydberg Series of Rb^{2+}

Using Equation (3), the energy resonances of the $4s^2 4p^4(^3P_1)nd$, $4s^2 4p^4(^1D_2)nd$ and $4s^2 4p^4(^1S_0)nd$ are given below (in Rydberg units).

- For the $4s^2 4p^5(^2P_{1/2}) \rightarrow 4s^2 4p^4(^3P_1)nd$ transition

$$E_n = E_\infty - \frac{1}{n^2} \left[Z - \sigma_1 - \sigma_2 \times \frac{1}{n} + \sigma_2 (n-m)(n-q) \left(\frac{1}{(n+m-3s)^2} - \frac{1}{(n+q-8s)^2} + \frac{1}{(n+q-m+7s)^3} \right) \right]^2 \tag{7}$$

- For the $4s^2 4p^5(^2P_{3/2}) \rightarrow 4s^2 4p^4(^3P_1)nd$ transition

$$E_n = E_\infty - \frac{1}{n^2} \left[Z - \sigma_1 - \sigma_2 \times \frac{1}{n} + \sigma_2 (n-m)(n-q) \left(\frac{1}{(n+m+s)^2} - \frac{1}{(n+q-s)^2} + \frac{1}{(n+q-m+9s)^3} \right) \right]^2 \tag{8}$$

- For the $4s^2 4p^5(^2P_{1/2}) \rightarrow 4s^2 4p^4(^1D_2)nd$ transition

$$E_n = E_\infty - \frac{1}{n^2} \left[Z - \sigma_1 - \sigma_2 \times \frac{1}{n} - \sigma_2 (n-m)(n-q) \left(\frac{1}{(n-m+2q-s)^2} + \frac{1}{(n+q-s)^2} + \frac{1}{(n+2q-s)^3} \right) \right]^2 \tag{9}$$

- For the $4s^2 4p^5(^2P_{3/2}) \rightarrow 4s^2 4p^4(^1D_2)nd$ transition

$$E_n = E_\infty - \frac{1}{n^2} \left[Z - \sigma_1 - \sigma_2 \times \frac{1}{n} - \sigma_2 (n-m)(n-q) \left(\frac{1}{(n+m-q+8s)^2} + \frac{1}{(n+q-m+2s)^2} + \frac{1}{(n+m-q+5s)^3} \right) \right]^2 \tag{10}$$

- For the $4s^24p^5(^2P^o_{1/2}) \rightarrow 4s^24p^4(^1S_0)nd$ transition

$$E_n = E_\infty - \frac{1}{n^2} \left[Z - \sigma_1 - \sigma_2 \times \frac{1}{n} + \sigma_2 (n-m)(n-q) \left(\frac{1}{(n+2q+5s)^2} + \frac{1}{(n+m)(n+q+3s)^2} - \frac{1}{(n+m+q+6s)^2} \right) \right]^2 \quad (11)$$

- For the $4s^24p^5(^2P^o_{3/2}) \rightarrow 4s^24p^4(^1S_0)nd$ transition

$$E_n = E_\infty - \frac{1}{n^2} \left[Z - \sigma_1 - \sigma_2 \times \frac{1}{n} - \sigma_2 (n-m)(n-q) \left(\frac{1}{(n+q+s)^2} + \frac{1}{(n+m+s)^2} + \frac{1}{(n-m+q+s)^3} \right) \right]^2 \quad (12)$$

To evaluate the σ -screen constants, we use the $E_{exp}(nd)$ experimental energy resonances and the E_∞ energy limits obtained by Macaluso *et al.* [5] [9]. We find:

- For the $4s^24p^5(^2P^o_{1/2}) \rightarrow 4s^24p^4(^3P_1)nd$ transition

Using $E_\infty = 39.109$ eV; $E_{exp}(13d) = 38.352$ eV ($m = 13$); $E_{exp}(14d) = 38.459$ eV ($q = 14$). Equation (7) gives $\sigma_1 = 34.023$ and $\sigma_2 = -1.164$

- For the $4s^24p^5(^2P^o_{3/2}) \rightarrow 4s^24p^4(^3P_1)nd$ transition

Using $E_\infty = 40.023$ eV; $E_{exp}(13d) = 39.268$ eV, $E_{exp}(14d) = 39.374$ eV ($m = 13$ and $q = 14$). Equation (8) gives $\sigma_1 = 34.003$ and $\sigma_2 = -0.855$

- For the $4s^24p^5(^2P^o_{1/2}) \rightarrow 4s^24p^4(^1D_2)nd$ transition

Using $E_\infty = 40.485$ eV; $E_{exp}(8d) = 38.446$ eV, $E_{exp}(9d) = 38.885$ eV ($m = 13$ and $q = 14$). Equation (9) gives $\sigma_1 = 33.999$ and $\sigma_2 = -0.767$

- For the $4s^24p^5(^2P^o_{3/2}) \rightarrow 4s^24p^4(^3P_1)nd$ transition

Using $E_\infty = 41.399$ eV; $E_{exp}(8d) = 39.347$ eV, $E_{exp}(8d) = 39.790$ eV ($m = 13$ and $q = 14$). Equation (10) gives $\sigma_1 = 34.000$ and $\sigma_2 = -0.852$

- For the $4s^24p^5(^2P^o_{1/2}) \rightarrow 4s^24p^4(^1S_0)nd$ transition

Using $E_\infty = 43.104$ eV; $E_{exp}(6d) = 39.332$ eV, $E_{exp}(7d) = 40.374$ eV ($m = 13$ and $q = 14$). Equation (11) gives $\sigma_1 = 34.006$ and $\sigma_2 = -0.992$

- For the $4s^24p^5(^2P^o_{3/2}) \rightarrow 4s^24p^4(^1S_0)nd$ transition

Using $E_\infty = 44.018$ eV; $E_{exp}(6d) = 40.242$ eV, $E_{exp}(7d) = 41.286$ eV ($m = 13$ and $q = 14$). Equation (12) gives $\sigma_1 = 34.008$ and $\sigma_2 = -1.014$

3. Results and Discussions

Our present results are listed in **Tables 1-6** and compared with the ALS experimental data of Macaluso *et al.* [5], the SCUNC calculations of Sakho *et al.* [7] and DARC calculations of McLaughlin and Babb [6]. Our results are expressed into eV (1 Ry = 0.5 a.u = 13.605698 eV) for direct comparison. The effective nuclear charge Z^* is calculated to validate the MAOT's analysis conditions in Equation (6). The analysis of the nuclear effective charge values indicates that the quantum defect values obtained along the calculations and quoted in **Tables 1-6** are also in agreement with the MAOT's conditions of Equation (6).

Table 1. Resonance Energy (E_n , eV), quantum defect (δ) and effective nuclear charge Z^* of the $4s^2 4p^4(^3P_1)nd$ Rydberg series converging to the $Rb^{3+} 4s^2 4p^4(^3P_1)$ threshold origin $Rb^{2+} 4s^2 4p^5(^2P_{1/2})$ metastable state. The present MAOT calculations are compared to the SCUNC calculations of Sakho *et al.* [7], DARC calculations of McLaughlin and Babb [6] and the ALS experimental measurements of Macaluso *et al.* [5]. $|\Delta E|$ denotes the energy difference between the MAOT calculations and the ALS measurements.

n	E_n (eV)				ΔE	δ				Z^*
	MAOT	SCUNC	ALS	DARC		MAOT	SCUNC	ALS	DARC	
13	38.352	38.352	38.352	38.348	0.000	0.28	0.28	0.28	0.31	3.066
14	38.459	38.458	38.459	38.449	0.000	0.27	0.28	0.28	0.31	3.060
15	38.545	38.544	38.544	38.543	0.001	0.27	0.28	0.28	0.30	3.054
16	38.615	38.614	38.614	38.612	0.001	0.26	0.28	0.28	0.30	3.049
17	38.672	38.671	38.671	38.670	0.001	0.26	0.28	0.28	0.30	3.047
18	38.720	38.719	38.719	38.718	0.001	0.26	0.28	0.28	0.31	3.044
19	38.761	38.760	38.760	38.759	0.001	0.24	0.28	0.28	0.30	3.039
20	38.795	38.794	38.794	38.794	0.001	0.25	0.28	0.28	0.28	3.038
21	38.825	38.824	38.824		0.001	0.24	0.28	0.28		3.034
22	38.850	38.850				0.26	0.28			3.033
23	38.873	38.872				0.22	0.28			3.032
24	38.892	38.891				0.24	0.28			3.031
25	38.909	38.909				0.26	0.28			3.031
26	38.925	38.924				0.23	0.28			3.024
27	38.938	38.938				0.24	0.28			3.022
28	38.950	38.950				0.25	0.28			3.021
29	38.961	38.961				0.24	0.28			3.020
30	38.971	38.970				0.21	0.28			3.019
31	38.980	38.979				0.24	0.28			3.018
32	38.988	38.987				0.24	0.28			3.017
33	38.995	38.995				0.23	0.28			3.016
34	39.002	39.001				0.27	0.28			3.015
35	39.008	39.007				0.28	0.28			3.014
36	39.013	39.013				0.24	0.28			3.013
37	39.019	39.018				0.23	0.28			3.012
38	39.023	39.023				0.26	0.28			3.012
39	39.028	39.027				0.22	0.28			3.012
40	39.032	39.031				0.23	0.28			3.010
41	39.035					0.24				3.010
42	39.039					0.25				3.010
43	39.042					0.25				3.009
44	39.045					0.26				3.009
45	39.048					0.24				3.009
-	-									-
-	-									-
∞	39.109					-				3.000

Table 2. Resonance Energy (E_n , eV), quantum defect (δ) and effective nuclear charge Z^* of the $4s^2 4p^4(^3P_1)nd$ Rydberg series converging to the $\text{Rb}^{3+} 4s^2 4p^4(^3P_1)$ threshold origin $\text{Rb}^{2+} 4s^2 4p^5(^2P_{3/2})$ ground state. The present MAOT calculations are compared to the SCUNC calculations of Sakho *et al.* [7], DARC calculations of McLaughlin and Babb [6] and the ALS experimental measurements of Macaluso *et al.* [9]. $|\Delta E|$ denotes the energy difference between the MAOT calculations and the ALS measurements.

n	$E_n(\text{eV})$				ΔE	δ				Z^*
	MAOT	SCUNC	ALS	DARC		MAOT	SCUNC	ALS	DARC	
13	39.268	39.268	39.268	39.263	0.000	0.26	0.26	0.27	0.31	3.062
14	39.374	39.374	39.374	39.379	0.000	0.26	0.26	0.27	0.32	3.058
15	39.459	39.459	39.459	39.457	0.000	0.27	0.26	0.27	0.32	3.054
16	39.529	39.529	39.528	39.526	0.001	0.26	0.26	0.27	0.30	3.049
17	39.586	39.586	39.586	39.584	0.000	0.26	0.26	0.27	0.30	3.047
18	39.634	39.634	39.634	39.632	0.000	0.26	0.26	0.27	0.32	3.044
19	39.675	39.674	39.674	39.673	0.001	0.24	0.26	0.27	0.30	3.039
20	39.709	39.709	39.709	39.707	0.000	0.25	0.26	0.27	0.30	3.038
21	39.739	39.738				0.23	0.26			3.034
22	39.764	39.764				0.26	0.26			3.033
23	39.787	39.786				0.22	0.26			3.032
24	39.806	39.806				0.24	0.26			3.031
25	39.824	39.823				0.23	0.26			3.024
26	39.839	39.838				0.23	0.26			3.024
27	39.852	39.852				0.24	0.26			3.023
28	39.864	39.864				0.24	0.26			3.023
29	39.875	39.875				0.24	0.26			3.022
30	39.885	39.885				0.24	0.26			3.021
31	39.894	39.893				0.23	0.26			3.019
32	39.902	39.901				0.23	0.26			3.018
33	39.909	39.909				0.23	0.26			3.018
34	39.916	39.915				0.23	0.26			3.015
35	39.922	39.922				0.23	0.26			3.015
36	39.928	39.927				0.23	0.26			3.015
37	39.933	39.932				0.23	0.26			3.015
38	39.937	39.937				0.24	0.26			3.015
39	39.942	39.941				0.24	0.26			3.015
40	39.946	39.945				0.24	0.26			3.015
41	39.950					0.24				3.015
42	39.953					0.24				3.013
43	39.956					0.25				3.013
44	39.959					0.26				3.013
45	39.962					0.24				3.013
-	-									-
-	-									-
∞	40.023					-				3.000

Table 3. Resonance Energy (E_n , eV), quantum defect (δ) and effective nuclear charge Z^* of the $4s^2 4p^4(^1D_2)nd$ Rydberg series converging to the $\text{Rb}^{3+} 4s^2 4p^4(^1D_2)$ threshold origin $\text{Rb}^{2+} 4s^2 4p^5(^2P_{1/2})$ metastable state. The present MAOT calculations are compared to the SCUNC calculations of Sakho *et al.* [7], DARC calculations of McLaughlin and Babb [6] and the ALS experimental measurements of Macaluso *et al.* [9]. $|\Delta E|$ denotes the energy difference between the MAOT calculations and the ALS measurements.

n	E_n (eV)				ΔE	δ				Z^*
	MAOT	SCUNC	ALS	DARC		MAOT	SCUNC	ALS	DARC	
8	38.446	38.446	38.446	38.440	0.000	0.25	0.25	0.25	0.26	3.097
9	38.885	38.885	38.885	38.884	0.000	0.25	0.25	0.25	0.25	3.086
10	39.197	39.196	39.196	39.192	0.001	0.25	0.25	0.25	0.26	3.077
11	39.425	39.425	39.425	39.424	0.000	0.25	0.25	0.25	0.26	3.070
12	39.598	39.598	39.598	39.597	0.000	0.25	0.25	0.25	0.26	3.064
13	39.732	39.732	39.731	39.731	0.001	0.25	0.25	0.25	0.26	3.058
14	39.838	39.838	39.837	39.837	0.001	0.24	0.25	0.25	0.26	3.053
15	39.923	39.922	39.922	39.922	0.001	0.24	0.25	0.25	0.26	3.049
16	39.992	39.992	39.991	39.991	0.001	0.24	0.25	0.25	0.26	3.046
17	40.050	40.049	40.048	40.048	0.002	0.22	0.25	0.25	0.26	3.040
18	40.097	40.097	40.096	40.096	0.001	0.24	0.24	0.25	0.26	3.040
19	40.138	40.137	40.136		0.002	0.21	0.24	0.25		3.034
20	40.172	40.171	40.171		0.001	0.22	0.24	0.25		3.033
21	40.202	40.201	40.200		0.002	0.20	0.24	0.25		3.029
22	40.227	40.226				0.21	0.24			3.030
23	40.249	40.249				0.22	0.24			3.029
24	40.269	40.268				0.22	0.24			3.024
25	40.286	40.285				0.22	0.24			3.023
26	40.301	40.300				0.21	0.24			3.023
27	40.315	40.314				0.21	0.24			3.018
28	40.327	40.326				0.21	0.24			3.017
29	40.338	40.337				0.24	0.24			3.014
30	40.347	40.347				0.21	0.24			3.022
31	40.356	40.356				0.24	0.24			3.018
32	40.364	40.364				0.22	0.24			3.018
33	40.371	40.371				0.23	0.24			3.021
34	40.378	40.371				0.23	0.24			3.015
35	40.384	40.384				0.22	0.24			3.016
36	40.390	40.389				0.22	0.24			3.008
37	40.395	40.394				0.24	0.24			3.008
38	40.400	40.399				0.24	0.24			3.008

Continued

39	40.404	40.403		0.22	0.24	3.008
40	40.408	40.408		0.22	0.24	3.008
41	40.412			0.25		3.008
42	40.415			0.24		3.008
43	40.418			0.24		3.008
44	40.421			0.25		3.008
45	40.424			0.24		3.008
-	-			-		-
-	-			-		-
∞	40.485			-		3.000

Table 4. Resonance Energy (E_n , eV), quantum defect (δ) and effective nuclear charge Z^* of the $4s^2 4p^4(^1D_2)nd$ Rydberg series converging to the $\text{Rb}^{3+} 4s^2 4p^4(^1D_2)$ threshold origin $\text{Rb}^{2+} 4s^2 4p^5(^2P_{3/2})$ ground state. The present MAOT calculations are compared to the SCUNC calculations of Sakho *et al.* [7], DARC calculations of McLaughlin and Babb [6] and the ALS experimental measurements of Macaluso *et al.* [9]. $|\Delta E|$ denotes the energy difference between the MAOT calculations and the ALS measurements.

n	$E_n(\text{eV})$				ΔE	δ				Z^*
	MAOT	SCUNC	ALS	DARC		MAOT	SCUNC	ALS	DARC	
8	39.347	39.347	39.347	39.355	0.000	0.28	0.28	0.28	0.26	3.107
9	39.790	39.789	39.790	39.797	0.000	0.28	0.28	0.28	0.26	3.095
10	40.104	40.104	40.104	40.109	0.000	0.28	0.28	0.28	0.26	3.085
11	40.335	40.334	40.334	40.339	0.001	0.27	0.28	0.28	0.26	3.076
12	40.509	40.508	40.508	40.511	0.001	0.27	0.27	0.28	0.26	3.069
13	40.644	40.643	40.643	40.645	0.001	0.26	0.27	0.28	0.26	3.062
14	40.751	40.749	40.749	40.751	0.002	0.25	0.27	0.28	0.26	3.055
15	40.836	40.835	40.834	40.836	0.002	0.25	0.27	0.28	0.26	3.051
16	40.906	40.904	40.904	40.905	0.002	0.25	0.27	0.28	0.26	3.046
17	40.963	40.962	40.961	40.962	0.002	0.25	0.27	0.28	0.26	3.043
18	41.011	41.009	41.009	41.010	0.002	0.25	0.27	0.28	0.26	3.040
19	41.051	41.050	41.050		0.001	0.25	0.27	0.28		3.039
20	41.086	41.084	41.084		0.002	0.26	0.27	0.28		3.033
21	41.115	41.114	41.114		0.001	0.26	0.27	0.28		3.034
22	41.141	41.140	41.140		0.001	0.26	0.27	0.28		3.030
23	41.163	41.162	41.162		0.001	0.26	0.27	0.28		3.029
24	41.183	41.182	41.182		0.001	0.26	0.27	0.28		3.024
25	41.200	41.199	41.199		0.001	0.26	0.27	0.28		3.023

Continued

26	41.215	41.214		0.26	0.27		3.023
27	41.229	41.228		0.26	0.27		3.018
28	41.241	41.240		0.26	0.27		3.017
29	41.252	41.251		0.25	0.27		3.014
30	41.261	41.260		0.25	0.27		3.014
31	41.270	41.269		0.25	0.27		3.014
32	41.278	41.277		0.25	0.27		3.014
33	41.285	41.285		0.25	0.27		3.013
34	41.292	41.291		0.25	0.27		3.013
35	41.298	41.297		0.25	0.27		3.012
36	41.304	41.303		0.25	0.27		3.012
37	41.309	41.308		0.25	0.27		3.012
38	41.314	41.313		0.25	0.27		3.012
39	41.318	41.317		0.25	0.27		3.012
40	41.322	41.321		0.25	0.27		3.012
41	41.326			0.26			3.012
42	41.329			0.26			3.010
43	41.332			0.26			3.010
44	41.335			0.26			3.010
45	41.338			0.26			3.010
-	-						-
-	-						-
∞	41.399			-			3.000

Table 5. Resonance Energy (E_n , eV), quantum defect (δ) and effective nuclear charge Z^* of the $4s^24p^4(^1S_0)nd$ Rydberg series converging to the $Rb^{3+} 4s^24p^4(^1S_0)$ threshold origin $Rb^{2+} 4s^24p^5(^2P_{1/2})$ metastable state. The present MAOT calculations are compared to the DARC calculations of McLaughlin and Babb [6] and the ALS experimental measurements of Macaluso *et al.* [9]. $|\Delta E|$ denotes the energy difference between the MAOT calculations and the ALS measurements.

n	E_n (eV)			ΔE	δ			Z^*
	MAOT	ALS	DARC		MAOT	ALS	DARC	
6	39.332	39.332	39.267	0.000	0.30	0.30	0.34	3.159
7	40.374	40.374	40.333	0.000	0.30	0.30	0.34	3.136
8	41.038	41.037	41.008	0.001	0.30	0.30	0.34	3.117
9	41.486	41.485	41.462	0.001	0.30	0.30	0.34	3.104
10	41.803	41.802	41.782	0.001	0.30	0.30	0.34	3.092
11	42.036	42.034	42.026	0.002	0.29	0.30	0.34	3.082

Continued

12	42.211	42.209	42.194	0.002	0.29	0.30	0.34	3.074
13	42.347	42.345	42.331	0.002	0.28	0.30	0.34	3.066
14	42.453	42.451	42.438	0.002	0.29	0.30	0.34	3.062
15	42.539	42.537	42.524	0.002	0.28	0.30	0.34	3.057
16	42.609	42.607	42.595	0.002	0.27	0.30	0.34	3.052
17	42.667	42.665		0.002	0.28	0.30		3.047
18	42.715	42.713		0.002	0.28	0.30		3.043
19	42.755	42.754		0.001	0.29	0.30		3.043
20	42.790	42.788		0.002	0.29	0.30		3.038
21	42.820	42.818		0.002	0.29	0.30		3.034
22	42.845				0.29	0.30		3.032
23	42.868				0.29			3.029
24	42.887				0.28			3.029
25	42.904				0.29			3.029
26	42.920				0.28			3.024
27	42.933				0.29			3.024
28	42.945				0.29			3.024
29	42.956				0.29			3.024
30	42.966				0.28			3.021
31	42.975				0.28			3.019
32	42.983				0.28			3.018
33	42.990				0.29			3.018
34	42.997				0.29			3.015
35	43.003				0.29			3.015
36	43.008				0.29			3.015
37	43.014				0.28			3.015
38	43.018				0.28			3.014
39	43.023				0.28			3.014
40	43.027				0.29			3.013
41	43.030				0.30			3.013
42	43.034				0.29			3.013
43	43.037				0.29			3.013
44	43.040				0.29			3.013
45	43.043				0.29			3.012
-	-							-
-	-							-
∞	43.104				-			3.000

Table 6. Resonance Energy (E_n , eV) and quantum defect (δ) and effective nuclear charge Z^* of the $4s^2 4p^4(^1S_0)nd$ Rydberg series converging to the $\text{Rb}^{3+} 4s^2 4p^4(^1S_0)$ threshold originating from $\text{Rb}^{2+} 4s^2 4p^5(^2P_{3/2})$ ground state. The present MAOT calculations are compared to the DARC calculations of McLaughlin and Babb [6] and the ALS experimental measurements of Macaluso *et al.* [9]. $|\Delta E|$ denotes the energy difference between the MAOT calculations and the ALS measurements.

n	$E_n(\text{eV})$			ΔE	δ			Z^*
	MAOT	ALS	DARC		MAOT	ALS	DARC	
6	40.242	40.242	40.182	0.000	0.31	0.31	0.34	3.161
7	41.286	41.286	41.248	0.000	0.31	0.31	0.34	3.137
8	41.949	41.950	41.922	0.001	0.31	0.31	0.34	3.120
9	42.397	42.398	42.376	0.001	0.31	0.31	0.34	3.107
10	42.713	42.715	42.697	0.002	0.31	0.31	0.34	3.097
11	42.946	42.947	42.931	0.001	0.31	0.31	0.34	3.088
12	43.122	43.127	43.108	0.005	0.31	0.31	0.34	3.079
13	43.254	43.258	43.245	0.004	0.31	0.31	0.34	3.072
14	43.362	43.365	43.353	0.003	0.31	0.31	0.34	3.067
15	43.449	43.451	43.439	0.002	0.30	0.31	0.34	3.062
16	43.520	43.521	43.509	0.001	0.30	0.31	0.34	3.058
17	43.578	43.579		0.001	0.30	0.31		3.054
18	43.628	43.627		0.001	0.29	0.31		3.048
19	43.667	43.668		0.001	0.29	0.31		3.047
20	43.703	43.702		0.001	0.29	0.31		3.043
21	43.733	43.732		0.001	0.29	0.31		3.040
22	43.759				0.29			3.036
23	43.781				0.29			3.036
24	43.801				0.30			3.031
25	43.818				0.30			3.031
26	43.833				0.31			3.032
27	43.847				0.31			3.027
28	43.859				0.30			3.027
29	43.870				0.30			3.025
30	43.880				0.30			3.021
31	43.889				0.30			3.019
32	43.897				0.30			3.018
33	43.904				0.30			3.021
34	43.911				0.30			3.015
35	43.927				0.30			3.016
36	43.923				0.30			3.009

Continued

37	43.928	0.30	3.010
38	43.932	0.31	3.021
39	43.937	0.31	3.009
40	43.941	0.31	3.010
41	43.945	0.30	3.003
42	43.948	0.30	3.013
43	43.951	0.30	3.018
44	43.954	0.31	3.018
45	43.957	0.30	3.014
-	-	-	-
-	-	-	-
∞	44.018	-	3.000

In **Table 1**, we quote the present MAOT results for resonance energies (E_n in eV), quantum defect (δ) and effective nuclear charge Z^* of the $4s^24p^4(^3P_1)nd$ Rydberg series relatively to the $4s^24p^5(^2P_{1/2})$ metastable state of Rb^{2+} . The results presented in this table are calculated by using the Equation (7). Thus, the maximum energy difference $|\Delta E|$ between the present calculations and the ALS experimental data of Macaluso *et al.* [5] is 0.001 eV. For $n = 13$ up to $n = 21$, we note a good agreement between results. For $n \geq 22$ up to $n = 40$, our results are compared with those of the SCUNC calculations of Sakho *et al.* [7]. For $n = 40$ our value at 39.032 eV is in good agreement with the SCUNC value at 39.031 eV. We also note that the nuclear effective charge Z^* and the quantum defect δ are in good agreement with the MAOT analysis conditions via Equation (6). This good agreement allows us to expect our results up to $n = 45$ to be accurate.

In **Table 2**, we report resonance energy (E_n in eV), quantum defect (δ) and effective nuclear charge Z^* of the $4s^24p^4(^3P_1)nd$ Rydberg series relatively to the $4s^24p^5(^2P_{3/2})$ ground state of Rb^{2+} . Results presented in this table are calculated via Equation (8). The agreements between the MAOT results and ALS experimental data are seen to be very good and the $|\Delta E|$ maximum energy difference is equal to 0.001 eV. For $n = 13 - 20$, we note a good agreement between results. For $n \geq 21$, our results are compared with the SCUNC results of Sakho *et al.* [7] that are the only known. Thus we note agreement between results and also the quantum defect agrees well with the analysis condition of Equation (6). This allows us to expect our resonance energies for this Rydberg series up to $n = 45$ to be accurate.

In **Table 3**, we present resonance energy (E_n in eV), quantum defect (δ) and effective nuclear charge Z^* of the $4s^24p^4(^1D_2)nd$ Rydberg series relatively to the $4s^24p^5(^2P_{1/2})$ metastable state of Rb^{2+} . Results presented in this table are calculated via Equation (9). for $n = 8 - 18$, we note agreement between our MAOT results and those of SCUNC [7], ALS [6] and DARC [9]. for $n = 21$, our MAOT value at 40.202 eV compare well with those of SCUNC and ALS at 40.201 eV and 40.200 eV re-

spectively. The maximum energy difference $|\Delta E|$ between our results and ALS experimental data of Macaluso *et al.* [9] is 0.002 eV. This slight discrepancies between the present calculations and experiment may be explained by the simplicity of the MAOT formalism which does not include explicitly any relativistic corrections. For $n \geq 22$ up to $n = 40$, our results are compared with the SCUNC results of Sakho *et al.* [7]. For $n = 40$, we note a good agreement for both methods values at 40.408 eV. In general agreements are seen to be very good between results and also the quantum defect agrees well with analysis condition of Equation (6). Thus for this Rydberg series, we can expect our results up to $n = 45$ to be accurate.

In **Table 4**, we quote results for resonance energy (E_n in eV), quantum defect (δ) and effective nuclear charge Z^* of the $4s^2 4p^4(^1D_2)nd$ Rydberg series relatively to the $4s^2 4p^5(^2P_{3/2})$ ground state of Rb^{2+} . Results presented in this table are calculated via Equation (10). For $n = 8 - 18$, our results are compared with those of Sakho *et al.* [7], of ALS experimental measurements of Macaluso *et al.* [9] and of DARC calculations of McLaughlin and Babb [6]. Agreements can be seen between results and the maximum energy difference between ALS experimental data of Macaluso *et al.* [5] and the present MAOT results is 0.002 eV. For $n = 19 - 25$, our Results are compared with the SCUNC results of Sakho [7] and DARC calculations of McLaughlin and Babb [6]. Thus, our value at 41.200 eV for $n = 25$ compares well with both results of the calculations at 41.199 eV and 41.199 eV respectively. The quantum defect and effective nuclear charge Z^* agree well with the MAOT analysis condition of Equation (6). These good agreements allow us to expect our MAOT results to be accurate for this Rydberg series.

We show in **Table 5** a comparison between our MAOT results and ALS measurements of Macaluso *et al.* [9] and DARC calculations of McLaughlin and Babb [6] for energy resonances (E_n in eV) and quantum defect (δ) of the $4s^2 4p^4(^1S_0)nd$ Rydberg series relatively to the $4s^2 4p^5(^2P_{1/2})$ metastable state of Rb^{2+} . Results presented in this table are calculated via Equation (11). From $n = 6$ up to $n = 16$, agreement is seen between results and for $n = 16$, our value at 42.609 eV compares well with ALS [9] and DARC [6] values respectively at 42.607 eV and 42.595 eV. Thus, this good agreement and the effective nuclear charge Z^* for MAOT's conditions analysis of Equation (6), allow us to continue our calculations up to $n = 21$ for direct comparison with ALS [9]. We also note the maximum $|\Delta E|$ energy difference is 0.002 eV and this good agreement allows to expect our results up to $n = 45$ to be accurate.

Table 6 presents resonance energies (E_n in eV), quantum defect (δ) and effective nuclear charge Z^* of the $4s^2 4p^4(^1S_0)nd$ Rydberg series relatively to the $4s^2 4p^5(^2P_{3/2})$ ground state of Rb^{2+} . Data tabulated here are only compared with those of DARC calculations of McLaughlin and Babb [6] and the ALS experimental data of Macaluso *et al.* [9]. Results presented in this table are calculated via Equation (12). The maximum $|\Delta E|$ energy difference between our MAOT calculations and ALS experimental data of Macaluso *et al.* [9] is to 0.005 eV corresponding to $n = 12$. The nuclear effective charge values allow us to expect our results on the resonance

energies for this Rydberg series up to $n = 45$ to be accurate. The slight discrepancies can be explained by the fact that, in the MAOT formalism, all the relativistic and electron correlation effects are implicitly taken into account in the adjustment parameters σ_i evaluated using experimental data.

4. Conclusion

In this paper, the Modified Atomic Orbital Theory (MAOT) is applied to report accurate resonance energies of the $4s^24p^4(^3P_1)nd$, $4s^24p^4(^1D_2)nd$ and $4s^24p^4(^1S_0)nd$ Rydberg series in the photoionization spectra originating from $4s^24p^5(^2P_{3/2})$ ground state and $4s^24p^5(^2P_{1/2})$ metastable state of Rb^{2+} . This work demonstrates the simplicity to use the MAOT semi-empirical procedure to calculate accurate energy values without excessive mathematical developments and tedious computer programming. The new accurate results in this paper are valuable and contribute directly to astrophysical research into Rb^{2+} nucleosynthesis. The slight discrepancies with experimental data may arise because the MAOT formalism does not explicitly include relativistic corrections. We have extended our results to $n = 45$ to provide new data for research. New data $n = 22 - 45$ for $4s^24p^4(^1S_0)nd$ Rydberg series originating from $4s^24p^5(^2P_{3/2})$ ground state and $4s^24p^5(^2P_{1/2})$ metastable state are tabulated for future Photoionization studies on Rb^{2+} focused on high excited levels.

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Credit Authors' Statement

Oumar Baba DIA: Conceptualization; Methodology, Software, Formal analysis, validation, Data curation, Writing—Original draft preparation; Writing—Reviewing and Editing, Validation.

Malick SOW: Conceptualization; Methodology, Formal analysis, validation, Data curation, Writing Original draft preparation; Writing—Reviewing and Editing, Validation.

Moustapha KEBE: Reviewing; Formal analysis, Validation.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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