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High Lying Precise Resonance Energies from Photoionization Studies of Se^{3+} and Rb^{+} Ions Using the Screening Constant per Unit Nuclear Charge Formalism

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Abstract: Resonance energies of the 4s4p ($^3P_{0,1}$)np, 4s4p ($^3P_2$)np ($^2P_{3/2}$, $^4D_{7/2}$, $^4D_{5/2}$) and 4s4p ($^1P_1$)np ($^2D_{3/2}$, $^2D_{5/2}$) Rydberg series of Se^{3+} ions along with resonance energies of the $4s^24p^5$ ($^2P^\circ_{1/2}$) nd $^1P^\circ_1$ and $4s4p^6$ ($^2S_{1/2}$) np $^1P^\circ_1$ series of Rb^+ ions are reported. Calculations are done in the framework of the screening constant per unit nuclear charge (SCUNC) formalism. The fine structure splitting of the 4s4p ($^3P_2$)np ($^2P_{3/2}$, $^4D_{7/2}$, $^4D_{5/2}$) series from n = 10 to n = 27 and for the 4s4p ($^1P_1$)np ($^2D_{3/2}$, $^2D_{5/2}$) series from n = 8 to 11 are resolved in this paper. Very good agreements are obtained between the present calculations and the available experimental and theoretical literature data. The present predicted data up to n = 40 may be of great importance for the atomic physics community in connection with the understanding of the chemical evolution of the Se and Rb elements in the Universe.

Keywords: photoionization; resonance energy; Rydberg series; fine structure splitting; SCUNC

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1. Introduction

Photoionization is the key phenomenon for understanding the chemical evolution of elements in the universe in connection with their abundances in photoionized astrophysical nebulae. For $Z > 30$, processes of neutron (n)-capture elements (e.g., Se, Kr, Br, Xe, Rb, Ba and Pb) produced by slow or rapid n-capture nucleosynthesis have been detected in a large number of ionized nebulae [1–4]. Intensive research has been made particularly on the photoionization of Kr, Br, Xe, Rb and of Se. As far as Kr and Xe elements are concerned, Bizau et al. [5] performed the first experiment on the photoionization spectrum of Kr^+ and Xe^+ in the energy range covering 15 eV above the first ionization threshold. McLaughlin and Balance [6] reported the first theoretical resonance energies of the $4s^24p^4$ ($^1D_2$)nd and $4s^24p^4$ ($^1S_0$)nd prominent Rydberg series observed in the photoionization spectra of Kr^+ and Xe^+ ions using the multi-channel R-matrix QB method of *Quigley–Berrington* (which defines matrices **Q** and **B** in terms of asymptotic solutions). In addition, using the Modified orbital atomic theory, Diop et al. [7], investigated the dominant Rydberg series of Halogen-like Kr^+ and Xe^+ ions. Moreover, Sakho [8] studied high lying ($^1D_2$, $^1S_0$) ns, nd Rydberg series in the photoionization spectra of the halogen-like ion Kr^+ in the framework of the screening constant per unit nuclear charge (SCUNC) method. On the other hand, active research has been performed on the photoionisation of Rb ions due to their importance for modeling astrophysical objects such as those in the asymptotic giant branch (AGB) region [9,10]. Photoionization study of Rb^{2+} ions is especially crucial because it permits to provide benchmark data allowing to aid in the formulation of so-called "ionization correction factors" used in the modeling of planetary nebula emission lines of Rb ions [11–13]. Macaluso et al. [14] performed high-resolution photoionization cross-section measurements for Rb^{2+} ions using synchrotron radiation and the photo-ion merged-beams technique. Following these measurements, McLaughlin and Babb [15] reported theoretical photoionization data for Rb^{2+} using the Dirac-Coulomb R-matrix approximation. Following the experimental [14] and theoretical [15] studies, Sakho [16] reported high lying photoionization data for Rb^{2+} ions in the framework of the SCUNC method. Moreover, Kilbane et al. [9] performed photoionisation measurements for Rb^{+} ions using both synchrotron radiation and dual laser plasma and compared their experimental data with the Hartree-Fock with exchange plus relativistic corrections calculations [9]. Afterward, McLaughlin and Babb [17] performed Dirac *R*-matrix calculations to report photoionization data compared with the earlier experimental and theoretical works [9]. On the other hand, photoionization of selenium ions such as Se^{+}, Se^{2+}, Se^{3+}, Se^{4+} and Se^{5+} were the subject of active research in connection with the understanding of the chemical evolution of Se in the universe. Photoionization of Se^{+} ions was pioneered experimentally by Esteves et al. [18] from the photo-ion merged-beams technique and theoretically by McLaughlin and Balance [19] who applied the Breit-Pauli and Dirac-Coulomb *R*-matrix approximations. In the same way, Sakho [20,21] reported high lying resonance energies belonging to numerous Rydberg series of Se^{+} using the SCUNC formalism. Furthermore, Esteves et al. [22] and Macaluso et al. [23] reported the first absolute single-photoionization cross-section measurements for Se^{3+} and Se^{5+} [22] and for Se^{2+} [23]. In the experiment of Esteves et al. [22] conducted at the Advanced Light Source (ALS) synchrotron radiation (SR) facility, fine structure splitting of the 4s4p $(^3P_2)np$ $(^2P_{3/2}, {}^4D_{7/2}, {}^4D_{5/2})$ and 4s4p $(^1P_1)np$ $(^2D_{3/2}, {}^2D_{5/2})$ series were unresolved and all the corresponding resonance energies overlap, respectively, for n = 10–27 and for n = 8–11. Furthermore, in the measurements of Kilbane et al. [9] and the calculations of McLaughlin and Babb [17], the resonance energies of the $4s^24p^5(^2P^{\circ}{}_{1/2})$ nd $^1P^{\circ}{}_1$ Rydberg series converging to the Rb^{2+} $(3d^{10}4s^24p^5\,{}^2P^{\circ}{}_{1/2})$ threshold were limited to low lying states n = 8–14 [9] and to n = 8–16 [17]. It should be underlined that, in the works of Kalyar et al. [24], precise wavelengths have been measured up to highly excited states n = 70 for the 4p $(^2P_{3/2}) \rightarrow nd$ $^2D_{3/2,5/2}$ and 4p $(^2P_{1/2}) \rightarrow nd$ $^2D_{3/2}$ transitions in K I. This particular example points out the importance of extending available low lying experimental measurements to highly excited energy levels. Very recently [25], the SCUNC formalism has been applied to the calculations of accurate transition energies and wavelengths belonging to the Rydberg transitions reported in Kalyar et al. [24] up to n = 100. The maximum shift in wavelengths relative to the experimental data [24] was at 0.03 nm up to n = 70. This points out the suitability of the SCUNC formalism to report accurate high resonance energies corresponding to high quantum number values as demonstrated in various previous studies [16,20,21,26]. The motivation of the present study is in this direction where we use the screening constant per unit nuclear charge method to report high lying precise resonance energies of the 4s4p $(^3P_2)np$ $(^2P_{3/2}, {}^4D_{7/2}, {}^4D_{5/2})$ and of the 4s4p $(^1P_1)np$ $(^2D_{3/2}, {}^2D_{5/2})$ Rydberg series of Se^{3+} ions and of the $4s^24p^5(^2P^{\circ}{}_{1/2})$ nd $^1P^{\circ}{}_1$ and $4s4p^6$ $(^2S_{1/2})$ np $^1P^{\circ}{}_1$ series of Rb^{+} ions. The paper is organized as follows. Section 2 presents a brief summary of SCUNC formalism. Section 3 presents a discussion of the results obtained and compared with the available literature data. In Section 4 we summarize and conclude the present study.

2. Theory

For a given Rydberg series originating from a-$^{2S+1}L_J$ state, we obtain [16,20,21,25]

$$E_n = E_\infty - \frac{Z^2}{n^2}\left[1-\beta(nl;s,\mu,\nu,{}^{2S+1}L^{\pi}.Z)\right]^2. \tag{1}$$

In this equation, ν and μ ($\mu > \nu$) denote the principal quantum numbers of the $(^{2S+1}L_J)$ nl Rydberg series used in the empirical determination of the f_k—screening constants, s represents the spin of the nl- electron ($s = \frac{1}{2}$), E_∞ is the energy value of the series limit, E_n denotes the resonance energy and Z stands for the atomic number (nuclear charge). The β-parameters are screening constants by unit nuclear charge expanded in inverse powers of Z and given by

$$\beta\left(Z, {}^{2S+1}L_J, n, s, \mu, \nu\right) = \sum_{k=1}^{q} f_k\left(\frac{1}{Z}\right)^k. \tag{2}$$

In Equation (2), $f_k = f_k(^{2S+1}L_J, n, s, \mu, \nu)$ are screening constants to be evaluated empirically and q stands for the number of terms in the expansion of the β–parameter. The resonance energy is in the general form

$$E_n = E_\infty - \frac{Z^2}{n^2}\left\{1 - \frac{f_1(^{2S+1}L_J^\pi)}{Z(n-1)} - \frac{f_2(^{2S+1}L_J^\pi)}{Z} \pm \sum_{k=1}^{q}\sum_{k'=1}^{q'} f_1^{k'} F(n,\mu,\nu,s) \times \left(\frac{1}{Z}\right)^k\right\}^2 \quad (3)$$

In Equation (3), $\pm\sum_{k=1}^{q}\sum_{k'=1}^{q'} f_1^{k'} F(n,\mu,\nu,s) \times \left(\frac{1}{Z}\right)^k$ is a corrective term introduced to stabilize the resonance energies by increasing the principal quantum number n.

In general, resonance energies are analyzed from the standard quantum-defect expansion formula

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

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

Besides, theoretical and measured energy positions can be analyzed by calculating the Z^*-effective nuclear charge in the framework of the SCUNC procedure. Let us then express the resonance energy as follows:

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

Comparing Equations (3) and (5), the effective nuclear charge is in the form

$$Z* = Z\left\{1 - \frac{f_1(^{2S+1}L^\pi)}{Z(n-1)} - \frac{f_2(^{2S+1}L^\pi)}{Z} \pm \sum_{k=1}^{q}\sum_{k'=1}^{q'} f_1^{k'} F(n,\mu,\nu,s) \times \left(\frac{1}{Z}\right)^k\right\}. \quad (6)$$

In addition, the f_2-parameter in Equation (3) can be theoretically determined from Equation (6) by neglecting the corrective term with the condition

$$\lim_{n\to\infty} Z* = Z\left(1 - \frac{f_2(^{2S+1}L^\pi)}{Z}\right) = Z_{core}. \quad (7)$$

So we get then:

$$f_2 = Z - Z_{\mathrm{core}} \quad (8)$$

The single photoionization process from an atomic X^{p+} system is given by

$$X^{p+} + h\nu \to X^{(p+1)+} + e^-. \quad (9)$$

Using (9), we find $Z_{\mathrm{core}} = p + 1$.

From Equations (4) and (5), we find the relationship between the effective nuclear charge and the quantum defect

$$\frac{Z^{2*}}{n^2} = \frac{Z_{core}^2}{(n-\delta)^2} \quad (10)$$

That means

$$Z* = \frac{Z_{core}}{\left(1 - \frac{\delta}{n}\right)}. \quad (11)$$

From the viewpoint of the SCUNC formalism, Equation (11) indicates clearly that, each Rydberg series must satisfy the following conditions

$$\begin{cases} Z* \geq Z_{core} \; if \; \delta \geq 0 \\ Z* \leq Z_{core} \; if \; \delta \leq 0 \\ \lim Z*_{n\to\infty} = Z_{core} \end{cases} \tag{12}$$

3. Results and Discussion

For the Se^{3+} and Rb^{+} ions considered in this work, Equation (9) is, respectively, in the form

$$Se^{3+} + h\nu \rightarrow Se^{4+} + e^{-}; Z_{core} = 4. \tag{13}$$

$$Rb^{+} + h\nu \rightarrow Rb^{2+} + e^{-}; Z_{core} = 2. \tag{14}$$

Equation (8) gives for Se^{3+}, $f_2 = 34 - 4 = 30$ and Rb^{+}, $f_2 = 37 - 2 = 35$.

The remaining f_1-parameters in Equation (3) are evaluated empirically from the experimental data of Esteves et al. [22] for Se^{3+} and of Kilbane et al. [9] for Rb^{+}. The results obtained are presented in the caption of each table. Tables 1 and 2 present comparisons of the resonance energies and quantum defects of the 4s4p ($^{3}P_{0,1}$)np Rydberg series originating from the $4s^24p$ $^{2}P_{1/2,3/2}$ states of Se^{3+} converging to the $^{3}P_{0,1}$ series limits in Se^{4+}. The agreements between the SCUNC results and the SR data [22] are seen to be very good up to n = 22. Almost constant quantum defects are obtained for both theory and experiment as revealed by the data quoted in Table 2. Tables 3 and 4 lists the resonance energies and quantum defects of the 4s4p ($^{3}P_2$)np ($^{2}P_{3/2}$, $^{4}D_{7/2}$, $^{4}D_{5/2}$) Rydberg series originating from the $4s^24p$ $^{2}P_{3/2}$ states of Se^{3+} converging to the $^{3}P_2$ series limit in Se^{4+}. The SCUNC results are compared with the SR measurements [22]. For n = 6–8, the SCUNC results agree well with the SR values [22]. For n = 9 up to n = 27, the fine structures splitting related to the 4s4p ($^{3}P_2$)np ($^{2}P_{3/2}$, $^{4}D_{7/2}$, $^{4}D_{5/2}$) Rydberg series are well resolved via the present calculations in contrast with the SR measurements [22]. Table 5 reports the resonance energies and quantum defects of the 4s4p ($^{1}P_1$)np ($^{2}D_{3/2}$, $^{2}D_{5/2}$) Rydberg series originating from the $4s^24p$ $^{2}P_{3/2}$ states of Se^{3+} converging to the $^{1}P_1$ series limit in Se^{4+}. It is seen that the SCUNC results compare very well with the SR measurements [22] for the low lying states n = 6–7. For n = 8–11, the SR resonances overlap. Here again, the resonance energies of the 4s4p ($^{1}P_1$)np ($^{2}D_{3/2}$, $^{2}D_{5/2}$) Rydberg series are well identified via the present SCUNC calculations up to n = 40. As stated by Esteves et al. [18], some resonances in their previous SR analysis were not resolved, either due to interference from other series or to limitations in photon energy resolution at high n values. Probable strong coupling series occur in the photoionisation processes of the Se^{+} ions. In any case, unresolved fine structure splitting may be explained by the interference from other series causing strong inter-series coupling and/or limitations in photon energy resolution. Table 6 lists the resonance energies and quantum defects of the $4s^24p^5$ ($^{2}P^{\circ}{}_{1/2}$) nd $^{1}P^{\circ}{}_1$ Rydberg series of Rb^{+} converging to the Rb^{2+} ($3d^{10}4s^24p^5$ $^{2}P^{\circ}{}_{1/2}$) threshold. The comparison indicates an excellent agreement between the present SCUNC results and the Dirac *R*-matrix calculations of McLaughlin and Babb [17] from n = 8 to n = 16. In addition, the SCUNC predictions agree very well with the synchrotron radiation (SR) and dual laser plasma (DPL) measurements of Kilbane et al. [9] up to n = 12. For n = 13, the shift in energy is at 0.02 eV. However, for n = 14, the SCUNC prediction and the Dirac *R*-matrix calculation [17] are, respectively, at 27.92 eV and 27.91 eV in contracts with the SR-DPL measurement equal to 27.95 eV. For n = 15, the SCUNC prediction and the Dirac *R*-matrix value [17] are equal to 27.95 eV and 27.91 eV in contracts with the SR-DPL measurement equal to 27.95 eV. As a result, the SR-DPL measurement at 27.95 eV for n = 14 may not be accurate and the theoretical data may be good references for this. The SR-DPL resonance energy at 27.95 eV may probably be that of the n = 15 level with the hypothesis that the SR-DPL line for n = 14 is unresolved. For n = 16–40, new SCUNC data are expected to be accurate are tabulated. It should be underlined that, for n = 13–14, the SR-DPL quantum defects are negative in contrast with the SCUNC predictions. To enlighten this point, one needs just to calculate the values of Z* using Equation (6). For the $4s^24p^5$ ($^{2}P^{\circ}{}_{1/2}$) nd $^{1}P^{\circ}{}_1$ series, Z* decreases towards Z_{core} = 2.0 from 2.0621 for the first entry $4s^24p^5$ ($^{2}P^{\circ}{}_{1/2}$) 8d $^{1}P^{\circ}{}_1$ to 2.0045 for the very higher $4s^24p^5$ ($^{2}P^{\circ}{}_{1/2}$) 100d $^{1}P^{\circ}{}_1$ level. This indicates clearly that $Z^* > Z_{core}$. Subsequently, positive quantum defects are allowed for the $4s^24p^5$ ($^2P^\circ{}_{1/2}$) *n*d $^1P^\circ{}_1$ Rydberg series as predicted by the SCUNC conditions analysis (12) of resonance energies. Finally, Table 7 presents the resonances energies of the $4s4p^6$ ($^2S_{1/2}$) *n*p $^1P^\circ{}_1$ Rydberg series of Rb^+ converging to the Rb^{2+} ($3d^{10}4s4p^6\,{}^2S_{1/2}$) threshold. For these series, the SCUNC results are seen to compare very well with the SR-DPL measurements of Kilbane et al. [9] along with the dual laser plasma (DPL) data of Neogi et al. [27] and corrected dual laser plasma (Coor-DPL) data of Neogi et al. [27] by Kilbane et al. [9] and with the Dirac *R*-matrix calculations of McLaughlin and Babb [17] for n = 5–7. It should be mentioned that there is an excellent agreement between the SCUNC prediction and the Coor-DPL [27] for n = 6. New SCUNC data are tabulated for n = 8–11.

Table 1. Resonance energies of the 4s4p ($^3P_{0,1}$)*n*p Rydberg series originating from the $4s^24p\ ^2P_{1/2,3/2}$ states of Se^{3+} converging to the $^3P_{0,1}$ series limits in Se^{4+}. The Screening constant per unit nuclear charge (SCUNC) results are compared to the synchrotron radiation (SR) measurements of Esteves et al. [22]. The screening constants are equal to: f_1 ($^2P_{3/2}$,$^3P_0$) = −6.579 ± 0.029, f_1 ($^2P_{3/2}$,$^3P_1$) = −7.303 ± 0.029 and f_1 ($^2P_{1/2}$,$^3P_1$) = −7.365 ± 0.029.

	$4s^24p\ ^2P_{3/2} \rightarrow$ 4s4p ($^3P_0$)*n*p		**$4s^24p\ ^2P_{3/2} \rightarrow$ 4s4p ($^3P_1$)*n*p**		**$4s^24p\ ^2P_{1/2} \rightarrow$ 4s4p ($^3P_1$)*n*p**	
n	**SCUNC**	**SR**	**SCUNC**	**SR**	**SCUNC**	**SR**
6	42.850	42.85	*below threshold*		42.950	42.95
7	46.335	46.35	46.170	46.17	46.691	46.82
8	48.380	48.40	48.339	48.33	48.880	48.96
9	49.666	49.70	49.702	49.70	50.247	50.29
10	50.524	-	50.609	50.63	51.154	51.26
11	51.125	51.12	51.242	51.26	51.785	51.79
12	51.562	51.55	51.699	51.71	52.243	52.27
13	51.890		52.041	52.06	52.585	52.62
14	52.142		52.304	52.31	52.847	52.88
15	52.340		52.509	52.53	53.052	53.07
16	52.498		52.673	52.68	53.216	53.22
17	52.627		52.806	52.81	53.349	53.36
18	52.733		52.915	52.92	53.458	53.46
19	52.822		53.006	53.01	53.549	53.53
20	52.896		53.083		53.626	53.63
21	52.959		53.148		53.691	53.70
22	53.014		53.203		53.746	53.75
23	53.061		53.251		53.794	
24	53.101		53.293		53.836	
25	53.137		53.329		53.872	
26	53.168		53.361		53.904	
27	53.196		53.390		53.933	
28	53.221		53.415		53.958	
29	53.243		53.437		53.980	
30	53.263		53.458		54.000	
31	53.280		53.476		54.019	
32	53.297		53.492		54.035	
33	53.311		53.507		54.050	
34	53.324		53.520		54.063	
35	53.336		53.533		54.075	
36	53.348		53.544		54.087	
37	53.358		53.554		54.097	
38	53.367		53.563		54.106	
39	53.376		53.572		54.115	
40	53.383		53.580		54.123	
…	…	…	…		…	
∞	53.530	53.530	53.728		54.271	

Table 2. Quantum defects (dimensionless) of the 4s4p ($^3P_{0,1}$)np Rydberg series originating from the $4s^24p$ $^2P_{1/2,3/2}$ states of Se^{3+} converging to the $^3P_{0,1}$ series limits in Se^{4+}. The SCUNC results are compared to the SR data of Esteves et al. [22].

	$4s^24p$ $^2P_{3/2}$ → 4s4p ($^3P_0$)np		$4s^24p$ $^2P_{3/2}$ → 4s4p ($^3P_1$)np		$4s^24p$ $^2P_{1/2}$ → 4s4p ($^3P_1$)np	
n	**SCUNC**	**SR**	**SCUNC**	**SR**	**SCUNC**	**SR**
6	1.49	1.49	*below threshold*		1.61	1.62
7	1.50	1.49	1.63	1.64	1.64	1.60
8	1.50	1.49	1.64	1.64	1.65	1.60
9	1.49	1.47	1.65	1.65	1.65	1.60
10	1.49	-	1.65	1.62	1.64	1.50
11	1.49	1.52	1.64	1.62	1.64	1.62
12	1.48	1.53	1.64	1.62	1.64	1.58
13	1.48		1.64	1.62	1.64	1.55
14	1.48		1.64	1.62	1.64	1.50
15	1.47		1.64	1.62	1.64	1.55
16	1.47		1.63	1.58	1.64	1.55
17	1.47		1.63	1.55	1.64	1.55
18	1.47		1.63	1.58	1.64	1.55
19	1.47		1.63	1.58	1.63	1.55
20	1.47		1.63		1.63	1.55
21	1.47		1.63		1.63	1.55
22	1.47		1.63		1.64	1.55
23	1.47		1.63		1.64	
24	1.47		1.63		1.64	
25	1.46		1.63		1.64	
26	1.46		1.63		1.64	
27	1.46		1.63		1.64	
28	1.46		1.63		1.64	
29	1.46		1.63		1.64	
30	1.46		1.63		1.64	
31	1.46		1.63		1.64	
32	1.46		1.63		1.64	
33	1.46		1.63		1.64	
34	1.46		1.63		1.64	
35	1.46		1.63		1.64	
36	1.46		1.63		1.64	
37	1.46		1.63		1.64	
38	1.46		1.63		1.64	
39	1.46		1.63		1.64	
40	1.46		1.63		1.64	

Table 3. Resonance energies (in eV) of the 4s4p ($^3P_2$)np ($^2P_{3/2}$, $^4D_{7/2}$, $^4D_{5/2}$) Rydberg series originating from the $4s^24p$ $^2P_{3/2}$ states of Se^{3+} converging to the $^3P_2$ series limit in Se^{4+}. The SCUNC results are compared to the SR data of Esteves et al. [22]. The screening constants are equal to: f_1 ($^3P_2$, $^2P_{3/2}$)) = −7.636 ± 0.029, f_1 ($^3P_2$, $^4D_{7/2}$) = −7.335 ± 0.027 and f_1 ($^3P_2$, $^2D_{5/2}$) = −6.982 ± 0.027.

	$4s^24p$ $^2P_{3/2}$ → 4s4p ($^3P_0$)np		4s4p ($^3P_2$)np ($^4D_{7/2}$)		4s4p ($^3P_2$)np ($^2D_{5/2}$)	
n	SCUNC	SR	SCUNC	SR	SCUNC	SR
6	42.640	42.64	42.890	42.89	43.180	43.18
7	46.592	46.51	46.731	46.75	46.891	46.90
8	48.810	48.82	48.894	48.86	48.992	48.92
9	50.179	50.19	50.234	50.19	50.298	50.24
10	51.083	51.18	51.121	51.18	51.165	51.18
11	51.712	51.71	51.739	51.71	51.771	51.71
12	52.167	52.20	52.187	52.20	52.210	52.20
13	52.507	52.53	52.522	52.53	52.540	52.53
14	52.767	52.77	52.779	52.77	52.793	52.77
15	52.972	52.97	52.981	52.97	52.992	52.97
16	53.135	53.13	53.142	53.13	53.151	53.13
17	53.267	53.26	53.273	53.26	53.281	53.26
18	53.376	53.37	53.381	53.37	53.387	53.37
19	53.466	53.46	53.471	53.46	53.476	53.46
20	53.543	53.53	53.546	53.53	53.551	53.53
21	53.607	53.60	53.610	53.60	53.614	53.60
22	53.663	53.66	53.665	53.66	53.669	53.66
23	53.7105	53.70	53.713	53.70	53.716	53.70
24	53.752	53.75	53.754	53.75	53.756	53.75
25	53.788	53.78	53.790	53.78	53.792	53.78
26	53.820	53.81	53.822	53.81	53.824	53.81
27	53.848	53.85	53.850	53.85	53.852	53.85
28	53.874		53.875		53.876	
29	53.896		53.897		53.898	
30	53.916		53.917		53.918	
31	53.934		53.935		53.936	
32	53.950		53.951		53.952	
33	53.965		53.966		53.967	
34	53.979		53.979		53.980	
35	53.991		53.991		53.992	
36	54.002		54.003		54.003	
37	54.012		54.013		54.013	
38	54.022		54.022		54.023	
39	54.030		54.031		54.031	
40	54.038		54.039		54.039	
…	…	…	…	…	…	…
∞	54.186	54.186	54.186	54.186	54.186	54.186

Table 4. Quantum defects (dimensionless) of the 4s4p ($^3P_2$)np ($^2P_{3/2}$, $^4D_{7/2}$, $^4D_{5/2}$) Rydberg series originating from the 4s^{2}4p $^2P_{3/2}$ states of Se^{3+} converging to the $^3P_2$ series limit in Se^{4+}. The SCUNC results are compared to the SR measurements of Esteves et al. [22].

	4s4p ($^3P_2$)np ($^2P_{3/2}$)		**4s4p ($^3P_2$)np ($^4D_{7/2}$)**		**4s4p ($^3P_2$)np ($^2D_{5/2}$)**	
n	**SCUNC**	**SR**	**SCUNC**	**SR**	**SCUNC**	**SR**
6	1.66	1.66	1.61	1.61	1.55	1.55
7	1.65	1.68	1.60	1.59	1.54	1.54
8	1.64	1.63	1.59	1.61	1.53	1.57
9	1.63	1.62	1.58	1.61	1.52	1.57
10	1.62	1.52	1.57	1.50	1.51	1.48
11	1.62	1.63	1.57	1.61	1.51	1.60
12	1.62	1.60	1.56	1.60	1.50	1.53
13	1.61	1.60	1.56	1.60	1.50	1.55
14	1.61	1.60	1.56	1.60	1.50	1.60
15	1.61	1.60	1.56	1.60	1.50	1.63
16	1.61	1.60	1.56	1.60	1.49	1.63
17	1.61	1.60	1.56	1.60	1.49	1.65
18	1.61	1.60	1.55	1.60	1.49	1.70
19	1.61	1.60	1.55	1.60	1.49	1.70
20	1.61	1.60	1.55	1.60	1.49	1.70
21	1.61	1.60	1.55	1.60	1.49	1.70
22	1.60	1.60	1.55	1.60	1.49	1.70
23	1.60	1.60	1.55	1.60	1.49	1.70
24	1.60	1.60	1.55	1.60	1.49	1.70
25	1.60	1.60	1.55	1.60	1.49	1.70
26	1.60	1.60	1.55	1.60	1.48	1.70
27	1.60	1.60	1.55	1.60	1.48	1.70
28	1.60		1.55		1.48	
29	1.60		1.55		1.48	
30	1.60		1.55		1.48	
31	1.60		1.55		1.48	
32	1.60		1.55		1.48	
33	1.60		1.55		1.48	
34	1.60		1.55		1.48	
35	1.60		1.55		1.48	
36	1.60		1.55		1.48	
37	1.60		1.55		1.48	
38	1.60		1.55		1.48	
39	1.60		1.55		1.48	
40	1.60		1.55		1.48	

Table 5. Resonance energies (in eV) and quantum defects (dimensionless) of the 4s4p ($^1P_1$)*n*p ($^2D_{3/2}$, $^2D_{5/2}$) Rydberg series originating from the $4s^24p$ $^2P_{3/2}$ states of Se^{3+} converging to the $^1P_1$ series limit in Se^{4+}. The SCUNC results are compared to the SR measurements of Esteves et al. [22]. The screening constants are equal to: f_1 ($^1P_1$, $^2D_{3/2}$) = −7.515 ± 0.028 and f_1 ($^1P_1$, $^2D_{5/2}$) = −7.362 ± 0.028.

	$4s^24p$ $^2P_{3/2}$ → $4s4p$ ($^1P_1$)np ($^2D_{3/2}$)				$4s^24p$ $^2P_{3/2}$ → $4s4p$ ($^1P_1$)np ($^2D_{5/2}$)			
	***E* (eV)**		**δ**		***E* (eV)**		**Δ**	
n	**SCUNC**	**SR**	**SCUNC**	**SR**	**SCUNC**	**SR**	**SCUNC**	**SR**
6	47.290	47.29	1.64	1.65	47.417	47.417	1.61	1.62
7	51.197	51.18	1.63	1.65	51.267	51.186	1.60	1.62
8	53.393	53.41	1.62	1.63	53.436	53.41	1.59	1.63
9	54.750	54.76	1.61	1.63	54.778	54.76	1.58	1.63
10	55.647	55.66	1.60	1.63	55.666	55.66	1.58	1.63
11	56.272	56.28	1.60	1.63	56.285	56.28	1.57	1.63
12	56.724		1.60		56.734		1.57	
13	57.062		1.59		57.070		1.56	
14	57.321		1.59		57.327		1.56	
15	57.524		1.59		57.529		1.56	
16	57.687		1.59		57.691		1.55	
17	57.819		1.59		57.822		1.55	
18	57.927		1.59		57.930		1.55	
19	58.017		1.59		58.019		1.55	
20	58.093		1.58		58.095		1.55	
21	58.158		1.58		58.159		1.55	
22	58.213		1.58		58.214		1.55	
23	58.260		1.58		58.262		1.55	
24	58.302		1.58		58.303		1.55	
25	58.338		1.58		58.339		1.55	
26	58.370		1.58		58.371		1.55	
27	58.398		1.58		58.399		1.55	
28	58.423		1.58		58.424		1.55	
29	58.445		1.58		58.446		1.55	
30	58.465		1.58		58.466		1.55	
31	58.483		1.58		58.484		1.55	
32	58.499		1.58		58.500		1.56	
33	58.514		1.58		58.515		1.56	
34	58.528		1.58		58.528		1.56	
35	58.540		1.58		58.540		1.56	
36	58.551		1.58		58.552		1.56	
37	58.561		1.58		58.562		1.56	
38	58.571		1.58		58.571		1.56	
39	58.579		1.58		58.580		1.57	
40	58.587		1.58		58.588		1.57	
...								
∞	58.735				58.735			

Table 6. Resonance energies (in eV) and quantum defects (dimensionless) of the $4s^24p^5$ ($^2P^\circ{}_{1/2}$) *n*d $^1P^\circ{}_1$ Rydberg series of Rb^+ converging to the Rb^{2+} ($3d^{10}4s^24p^5\,{}^2P^\circ{}_{1/2}$) threshold. The present SCUNC results are compared to the synchrotron radiation (SR) and dual laser plasma (DPL) measurements of Kilbane et al. [9] along with their theoretical results from Hartree-Fock with exchange plus relativistic corrections (HXR) [9] and with the Dirac *R*-matrix calculations of McLaughlin and Babb [17]. The SCUNC screening constant is f_1 ($^2P^\circ{}_{1/2}$, $^1P^\circ{}_1$) = −0.435 ± 0.028.

	Resonance Energies E_n				**Quantum Defects δ_n**			
n	**SCUNC**	***R*-Matrix**	**SR-DPL**	**HXR**	**SCUNC**	***R*-Matrix**	**SR-DPL**	**HXR**
8	27.3000	27.3008	27.30	27.3099	0.2411	0.2376	0.1977	0.1982
9	27.4949	27.4805	27.50	27.4595	0.2391	0.3265	0.2077	0.3922
10	27.6330	27.6223	27.63	27.5900	0.2375	0.3257	0.2628	0.5853
11	27.7343	27.7263	27.74	27.6814	0.2362	0.3253	0.1699	0.7952
12	27.8108	27.8046	27.82	27.7519	0.2351	0.3246	0.0951	1.0283
13	27.8700	27.8652	27.89	27.8072	0.2342	0.3243	−0.1651	1.2887
14	27.9168	27.9129	27.95	27.8515	0.2334	0.3241	−0.6377	1.5846
15	27.9544	27.9512			0.2327	0.3239		
16	27.9851	27.9824			0.2321	0.3239		
17	28.0104				0.2316			
18	28.0316				0.2312			
19	28.0495				0.2308			
20	28.0648				0.2304			
21	28.0778				0.2301			
22	28.0892				0.2298			
23	28.0990				0.2295			
24	28.1077				0.2293			
25	28.1153				0.2290			
26	28.1221				0.2288			
27	28.1281				0.2286			
28	28.1334				0.2285			
29	28.1383				0.2283			
30	28.1426				0.2281			
31	28.1465				0.2280			
32	28.1501				0.2279			
33	28.1533				0.2277			
34	28.1563				0.2276			
35	28.1590				0.2275			
36	28.1615				0.2274			
37	28.1638				0.2273			
38	28.1659				0.2272			
39	28.1678				0.2271			
40	28.1696				0.2271			
…	…							
∞	28.204	28.204	28.204	28.204				

Table 7. Resonance energies (in eV) of the $4s4p^6$ ($^2S_{1/2}$) np $^1P°_1$ Rydberg series of Rb^+ converging to the Rb^{2+} ($3d^{10}4s4p^6$ $^2S_{1/2}$) threshold. The SCUNC results are compared to the synchrotron radiation (SR) and dual laser plasma (DPL) measurements of Kilbane et al. [9] along with the dual laser plasma (DPL) data of Neogi et al. [26] and corrected dual laser plasma (Coor-DPL) data of Neogi et al. [26] by Kilbane et al. [9] and with the Dirac *R*-matrix calculations of McLaughlin and Babb [17]. The screening constant f_1 ($^2S_{1/2}$, $^1P°_1$) = −7.255 ± 0.020.

n	SCUNC	*R*-Matrix	Corr-DPL	SR-DPL	DPL
5	35.714	35.720	35.714	35.708	35.710 ± 0.02
6	39.436	39.448	39.436	39.442	
7	40.933	40.942			
8	41.659				
9	42.025				
10	42.193				
11	42.241				

4. Summary and Conclusions

In this paper, accurate resonance energies of the 4s4p ($^3P_{0,1}$)np, 4s4p ($^3P_2$)np ($^2P_{3/2}$, $^4D_{7/2}$, $^4D_{5/2}$) and 4s4p ($^1P_1$)np ($^2D_{3/2}$, $^2D_{5/2}$) Rydberg series of Se^{3+} and of the $4s^24p^5$ ($^2P°_{1/2}$) nd $^1P°_1$ and $4s4p^6$ ($^2S_{1/2}$) np $^1P°_1$ series of Rb^+ are reported in the framework of the screening constant per unit nuclear charge formalism. Overall, very good agreements are obtained between the SCUNC predictions and the available literature data. In addition, the possibility to use the SCUNC method to resolve unresolved fine structure splitting measurements is demonstrated in this paper as far as the 4s4p ($^3P_2$)np ($^2P_{3/2}$, $^4D_{7/2}$, $^4D_{5/2}$) and 4s4p ($^1P_1$)np ($^2D_{3/2}$, $^2D_{5/2}$) series are concerned. The new SCUNC values up to n = 40 may be useful photoionization data for incorporation into astrophysical modeling codes in connection with the understanding of the chemical evolution of Se and Kb elements in the Universe.

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References

1. Sharpee, B.; Zhang, Y.; Williams, R.; Pellegrini, E.; Cavagnolo, K.; Baldwin, J.A.; Phillips, M.; Liu, X.W. s-Process Abundances in Planetary Nebulae. *Astrophys. J.* **2007**, *659*, 1265. [CrossRef]
2. Pequignot, D.; Baluteau, J.P. The identification of krypton, xenon, and other elements of rows 4, 5 and 6 of the periodic table in the planetary nebula NGC 7027. *Astron. Astrophys.* **1994**, *283*, 593–625.
3. Sterling, N.C.; Dinerstein, H.L.; Kallman, T.R. The abundances of light neutron-capture elements in planetary nebulae. I. Photoionization modeling and ionization corrections. *Astrophys. J. Suppl. Ser.* **2007**, *169*, 37. [CrossRef]
4. Sterling, N.C.; Dinerstein, H.L. The abundances of light neutron-capture elements in planetary nebulae. II. s-process enrichments and interpretation. *Astrophys. J. Suppl. Ser.* **2008**, *174*, 157. [CrossRef]
5. Bizau, J.M.; Blancard, C.; Coreno, M.; Cubaynes, D.; Dehon, C.; El Hassan, N.; Folkmann, F.; Gharaibeh, M.F.; Giuliani, A.; Lemaire, J.; et al. Photoionization study of Kr^+ and Xe^+ ions with the combined use of a merged-beam set-up and an ion trap. *J. Phys. B At. Mol. Opt. Phys.* **2011**, *44*, 055205. [CrossRef]
6. McLaughlin, B.M.; Ballance, C.P. Photoionization cross section calculations for the halogen-like Kr^+ and Xe^+. *J. Phys. B At. Mol. Opt. Phys.* **2012**, *45*, 085701. [CrossRef]
7. Diop, B.; Faye, M.; Dieng, M.; Sow, M.; Guèye, M.; Sakho, I.; Biaye, M.; Wagué, A. Modified Orbital Atomic Study of Dominant Rydberg series in the Photoionization Spectra of Halogen-like Kr^+ and Xe^+ ions. *Chin. J. Phys.* **2014**, *52*, 1223.
8. Sakho, I. Screening Constant by Unit Nuclear Charge Calculations of High lying Energy resonances in the Photoionization Spectra of Halogen-like Kr^+ ion. *At. Data. Nuc. Data Tables* **2014**, *100*, 297. [CrossRef]
9. Kilbane, D.; Folkmann, F.; Bizau, J.-M.; Banahan, C.; Scully, S.; Kjeldsen, H.; van Kampen, P.; Mansfield, M.W.D.; Costello, J.T.; West, J.B. Absolute photoionization cross-section measurements of the Kr I isoelectronic sequence. *Phys. Rev. A* **2007**, *75*, 032711. [CrossRef]
10. Sneden, C.; Gratton, R.G.; Crocker, D.A. Trends in copper and zinc abundances for disk and halo stars. *Astron. Astrophys.* **1991**, *246*, 354.

11. Langanke, K.; Wiescher, M. Nuclear reactions and stellar processes. *Rep. Prog. Phys.* **2001**, *64*, 1657–1701. [CrossRef]
12. Kwitter, K.B.; Méndez, R.H.; Peña, M.; Stanghellini, L.; Corradi, R.L.M.; De Marco, O.; Fang, X.; Henry, R.B.C.; Karakas, A.I.; Liu, X.-W.; et al. The present and future of planetary nebula research. A white paper by the IAU planetary nebula working group. *Rev. Mex. Astron. Astrofísica* **2014**, *50*, 203.
13. Luridiana, V.; Morisset, C.; Shaw, R.A. PyNeb: A new tool for analyzing emission lines I. Code description and validation of results. *Astron. Astrophys.* **2015**, *573*, A42. [CrossRef]
14. Macaluso, D.A.; Bogolub, K.; Johnson, A.; Aguilar, A.; Kilcoyne, A.; Bilodeau, R.C.; Bautista, M.; Kerlin, A.B.; Sterling, N.C. Absolute single photoionization cross-section measurements of Rb^{2+} ions: Experiment and theory. *J. Phys. B At. Mol. Opt. Phys.* **2017**, *50*, 119501. [CrossRef]
15. McLaughlin, B.M.; Babb, J.F. Photoionization of Rb^{2+} ions in the valence energy region 37–44 eV. *J. Phys. B At. Mol. Opt. Phys.* **2019**, *52*, 125201. [CrossRef]
16. Sakho, I. Screening Constant by Unit Nuclear Charge Photoionization of Rb^{2+} Ions. *J. At. Mol. Condens. Nano Phys.* **2019**, *6*, 69.
17. McLaughlin, B.M.; Babb, J.F. Single photoionization of the Kr-like Rb ii ion in the photon energy range 22–46.0 eV. *Mon. Not. R. Astron. Soc.* **2019**, *486*, 245–250. [CrossRef]
18. Esteves, D.A.; Bilodeau, R.C.; Sterling, N.C.; Phaneuf, R.A.; Kilcoyne, A.L.D.; Red, E.C.; Aguilar, A. Absolute high-resolution Se+ photoionization cross-section measurements with Rydberg-series analysis. *Phys. Rev. A.* **2011**, *84*, 013406. [CrossRef]
19. McLaughlin, B.M.; Ballance, C.P. Photoionization cross sections for the trans-iron element $Se^{+}$from 18 to 31 eV. *J. Phys. B At. Mol. Opt. Phys.* **2012**, *45*, 095202. [CrossRef]
20. Sakho, I. Calculations of high-lying energy resonances of the $4s^24p^2$ $(^1D_2)$nd and $4s^24p^2$ $(^1S_0)$nd Rydberg series of Se^{+}. *Phys. Rev. A* **2012**, *86*, 052511. [CrossRef]
21. Sakho, I. Screening Constant per Unit Nuclear Charge Studies of Rydberg Resonances Due to the 4p $\rightarrow$ *nd* and *ns* Transitions in Se+ Ions. *Atoms* **2022**, *10*, 107. [CrossRef]
22. Esteves, D.A.; Bilodeau, R.C.; Phaneuf, R.A.; Kilcoyne, A.L.D.; Red, E.C.; Aguilar, A.; Sterling, N.C. Absolute photoionization cross-section measurements of Se^{3+} and Se^{5+}. *J. Phys. B At. Mol. Opt. Phys.* **2012**, *45*, 115201. [CrossRef]
23. Macaluso, D.A.; Aguilar, A.; Kilcoyne, A.L.D.; Red, E.C.; Bilodeau, R.C.; Phaneuf, R.A.; Sterling, N.C.; McLaughlin, B.M. Absolute single-photoionization cross sections of Se^{2+}: Experiment and theory. *Phys. Rev. A* **2015**, *92*, 063424. [CrossRef]
24. Kalyar, M.A.; Yar, A.; Ali, R.; Baig, M.A. Measurements of photoionization cross section of the 4p levels and oscillator strength of the 4p$\rightarrow$*n*d $^2D_{3/2,5/2}$ transitions of potassium. *Opt. Laser Technol.* **2016**, *77*, 72. [CrossRef]
25. Sakho, I. Study of single-photon photoionization of oxygen-like Ne III via the screening constant per unit nuclear charge. *Int. J. Mass Spectrom.* **2022**, *474*, 116800. [CrossRef]
26. Sakho, I. Precise wavelengths of the 4p $(^2P_{1/2}) \rightarrow n$d $^2D_{3/2}$ and 4p $(^2P_{3/2}) \rightarrow n$d $^2D_{3/2,5/2}$ Rydberg transitions in neutral potassium calculated via the Screening Constant per Unit nuclear Charge method. Zhurnal Prikladnoi Spektroskopii (ZhPS). *J. Appl. Spectrosc.* **2023**, *90*, 3.
27. Neogi, A.; Kennedy, E.T.; Mosnier, J.P.; van Kampen, P.; Costello, J.T.; O'Sullivan, G.; Mansfiled, M.W.D.; Demekhin, P.V.; Lagutin, B.M.; Sukhorukov, V.L. Trends in autoionization of Rydberg states converging to the 4s threshold in the $Kr-Rb^{+}-Sr^{2+}$ isoelectonic sequence: Theory and experiment. *Phys. Rev. A* **2003**, *67*, 042707. [CrossRef]