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Photoionization of Rb^{2+} Ions Using the Screening Constant by Unit Nuclear Charge Formalism

Research Article

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Abstract. We report in this paper Photoionization data of the Rb^{2+} ions. Rydberg series of resonances due to $4p \rightarrow nd$ transitions from the $^2P^\circ_{3/2}$ ground state and the $^2P^\circ_{1/2}$ metastable state of Rb^{2+} converging to the $4s^2 4p^4$ ($^1D_2$) series limit in Rb^{3+} are considered. Calculations are performed in the framework of the *Screening Constant by Unit Nuclear Charge* (SCUNC) formalism and accurate data are tabulated up to $n = 40$. It is shown that the SCUNC analytical formulas reproduce with an excellent precision, recent ALS measurements of Macaluso et al. [*J. Phys. B: At. Mol. Opt. Phys*. **50** (2017)]. New data are tabulated for $n = 25$-40.

Keywords. Photoionization; Rydberg series; Ground state; Metastable state; SCUNC

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1. Introduction

Photoionization studies of Rb ions [1–3] remain an active field of investigations due to their importance for modeling astrophysical objects such those in the *Asymptotic Giant Branch* (AGB) region. It is widely believed that, a major source of discrepancy is the quality of the atomic data used in the modelling [4–6, 8]. Recently, Macaluso et al. [9] performedhigh-resolution measurements of the photoionization cross section of Rb^{2+}using synchrotron radiation and the photo-ion, merged-beams technique at the Advanced Light Source at Lawrence Berkeley National Laboratory. The motivation of this work is to use the *Screening Constant by Unit*

Nuclear Charge (SCUNC) formalism [10–12] to report high lying Photoionization data of the Rb^{2+} ions to be compared to the high-resolution measurements [9]. The layout of this work is as follows. Section 2 presents a brief outline of the theoretical part of the work. Section 3 presents a discussion of the results obtained compared with the available literature data. Finally, in Section 4 we summarize and conclude the present study.

2. Theory

In the framework of the Screening Constant by Unit Nuclear Charge formalism, the total energy of the $(Nl, nl')^{2S+1}L^{\pi}$ excited states is expressed in the form (in Rydberg)

$$E = -Z^2\left(\frac{1}{N^2} + \frac{1}{n^2}\left[1-\beta\left(Nl, nl'^{2S+1}L^{\pi}; Z\right)\right]^2\right). \tag{2.1}$$

In this equation, the principal quantum numbers N and n are respectively for the inner and the outer electron of the helium-isoelectronic series. The β-parameters are screening constants by unit nuclear charge expanded in inverse powers of Z and given by

$$\beta\left(Nl\,nl'; {}^{2S+1}L^{\pi}; Z\right) = \sum_{k=1}^{q} f_k\left(\frac{1}{Z}\right)^k \tag{2.2}$$

where $f_k = f_k\left(Nl\,nl'; {}^{2S+1}L^{\pi}\right)$ are parameters to be evaluated empirically.

For a given Rydberg series originating from a-$^{2S+1}L_J$ state, we obtain using [10–12]

$$E_n = E_\infty - \frac{Z^2}{n^2}\left[1-\beta(nl; s, \mu, \nu, {}^{2S+1}L^{\pi}.Z)\right]^2. \tag{2.3}$$

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. The β-parameters are screening constants by unit nuclear charge expanded in inverse powers of Z and given by

$$\beta(Z, {}^{2S+1}L_J, n, s, \mu, \nu) = \sum_{k=1}^{q} f_k\left(\frac{1}{Z}\right)^k \tag{2.4}$$

where $f_k = f_k({}^{2S+1}L_J, n, s, \mu, \nu)$ are screening constants to be evaluated empirically. In eq. (2.2), q stands for the number of terms in the expansion of the β-parameter. The resonance energy are the in the form

$$E_n = E_\infty - \frac{Z^2}{n^2}\left\{1 - \frac{f_1({}^{2S+1}L_J^{\pi})}{Z(n-1)} - \frac{f_2({}^{2S+1}L_J^{\pi})}{Z} \pm \sum_{k=1}^{q}\sum_{k'=1}^{q'} f_1^{k'} F(n,\mu,\nu,s)\times\left(\frac{1}{Z}\right)^k\right\}^2. \tag{2.5}$$

In this equation, $\pm\sum_{k=1}^{q}\sum_{k'=1}^{q'} f_1^{k'} F(n,\mu,\nu,s)\times\left(\frac{1}{Z}\right)^k$ is a corrective term introduce to stabilize the resonance energies with increasing the principal quantum number n. In general, resonance energies are analyzed from the standard quantum-defect expansion formula

$$E_n = E_\infty - \frac{RZ_{\text{core}}^2}{(n-\delta)^2}. \tag{2.6}$$

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 means the quantum defect. In addition, theoretical and measured energy positions can be analyzed by calculating the Z^*-effective charge in the framework of the SCUNC-procedure

$$E_n = E_\infty - \frac{Z^{*2}}{n^2} R. \tag{2.7}$$

The relationship between Z^* and δ is in the form

$$Z^* = \frac{Z_{\text{core}}}{\left(1 - \frac{\delta}{n}\right)}. \tag{2.8}$$

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

$$\begin{cases} Z^* \geq Z_{\text{core}} & \text{if } \delta \geq 0 \\ Z^* \leq Z_{\text{core}} & \text{if } \delta \leq 0 \\ \lim\limits_{n\to\infty} Z^* = Z_{\text{core}} & \end{cases} \tag{2.9}$$

Besides, comparing eq. (2.5) and eq. (2.7), the effective charge is in the form

$$Z* = Z\left\{1 - \frac{f_1(^{2S+1}L^\pi)}{Z(n-1)} - \frac{f_2(^{2S+1}L^\pi)}{Z} \pm \sum_{k=1}^{q}\sum_{k'=1}^{q'} f_1^{k'} F(n,\mu,\nu,s) \times \left(\frac{1}{Z}\right)^k\right\}. \tag{2.10}$$

Besides, the f_2-parameter in eq. (2.2) can be theoretically determined from eq. (2.10) by neglecting the corrective term with the condition

$$\lim_{n\to\infty} Z* = Z\left(1 - \frac{f_2(^{2S+1}L^\pi)}{Z}\right) = Z_{\text{core}}. \tag{2.11}$$

We get then $f_2 = Z - Z_{\text{core}}$, where Z_{core} is directly obtain by the photoionization process from an atomic X^{p+} system $X^{p+} + h\nu \to X^{(p+1)+} + e^-$. We find then $Z_{\text{core}} = p + 1$. So, for the Rb^{2+} ions, $Z_{\text{core}} = 3$ and $f_2 = (37 - 3) = 34.0$. The remaining f_1-parameter is to be evaluated empirically using the ALS data of Macaluso et al. [9] for a given $(^{2S+1}L_J)\ \mu l$ level with $\nu = 0$. The empirical procedure of the determination of the f_1-screening constant along with the corresponding uncertainty have been explained in details in our previous work [10–12]. In the present work, all the energy resonances are calculated using the following simple expression

$$E_n = E_\infty - \frac{Z^2}{n^2}\left\{1 - \frac{f_1(^2D_2)}{Z(n-1)} - \frac{34.0}{Z} - \frac{f_1(^2D_2)(n-\mu)}{Z^2(n+\mu+s)(n-\mu+s)} - \frac{f_1(^2D_2)(n-\mu)^2}{Z^3(n+\mu+s)(n-\mu+s)}\right\}^2. \tag{2.12}$$

3. Results and Discussion

The ALS measurements of Macaluso et al. [9] were made at a photon energy resolution of 13.5 ± 2.5 meV from 37.31 to 44.08 eV spanning the $^2P^\circ{}_{3/2}$ ground state and $^2P^\circ{}_{1/2}$ metastable state ionization thresholds. These authors compared their measurements to Breit-Pauli R-matrix calculations and found excellent agreement between theory and experiment. The present SUCNC calculations are compared to the corrigendum work [9] where formatting errors occurred in the first paper [13] have been corrected. Comparison of the data quoted in Tables 1-2 show an excellent agreement between the SCUNC predictions and the ALS measurements [9]. In should be mentioned that all the SCUNC data are obtained from the single formula (2.12). Besides analysis of the data in view of Z^* indicate that $Z^*_{\text{max}} > Z_{\text{core}} = 3.0$.

According to the SCUNC analysis (2.9), the quantum defect is positive. This is what one can observe for both the SCUNC and ALS data presented in Tables 1-2. In addition, for n infinite, $Z^* = Z_{\text{core}} = 3.0$ as indicated in the last lines of Tables 1-2. This means that the PI of Rb^{2+} leads indeed to the Rb^{3+} ions.

Table 1. Energy resonances (E_n, eV), quantum defect (δ) and effective nuclear charge Z^* of the Rydberg series due to $4p \to nd$ transitions from the $^2P°_{3/2}$ ground state of Rb^{2+} converging to the $4s^24p^4$ ($^1D_2$) series limit in Rb^{3+}

	f_1 ($^2D_2$;$^2P°_{3/2}$) = −0.980 ± 0.080; μ = 8					f_1 ($^2D_2$;$^2P°_{3/2}$) = −0.748 ± 0.080; μ = 8				
	SCUNC	ALS	SCUNC	ALS	SCUNC	SCUNC	ALS	SCUNC	ALS	SCUNC
n	E_n	E_n	δ	δ	Z^*	E_n	E_n	δ	δ	Z^*
8	39.3030	39.303	0.357	0.357	3.141	39.3470	39.347	0.275	0.275	3.107
9	39.7602	39.761	0.356	0.357	3.125	39.7907	39.790	0.274	0.275	3.094
10	40.0830	40.082	0.354	0.357	3.111	40.1049	40.104	0.272	0.275	3.084
11	40.3189	40.318	0.352	0.357	3.100	40.3352	40.334	0.271	0.275	3.076
12	40.4966	40.496	0.351	0.357	3.091	40.5091	40.508	0.270	0.275	3.069
13	40.6338	40.633	0.350	0.357	3.084	40.6435	40.643	0.269	0.275	3.063
14	40.7419	40.741	0.349	0.357	3.077	40.7496	40.749	0.268	0.275	3.059
15	40.8286	40.828	0.348	0.357	3.072	40.8349	40.834	0.267	0.275	3.054
16	40.8992	40.899	0.347	0.357	3.067	40.9043	40.904	0.266	0.275	3.051
17	40.9575	40.957	0.347	0.357	3.063	40.9617	40.961	0.266	0.275	3.048
18	41.0061	41.006	0.346	0.357	3.059	41.0097	41.009	0.266	0.275	3.045
19	41.0471	41.047	0.346	0.357	3.056	41.0501	41.050	0.265	0.275	3.042
20	41.0820	41.082	0.346	0.357	3.053	41.0846	41.084	0.265	0.275	3.040
21	41.1120	41.112	0.345	0.357	3.051	41.1142	41.114	0.265	0.275	3.038
22	41.1379	41.138	0.345	0.357	3.048	41.1398	41.140	0.264	0.275	3.037
23	41.1604	41.160	0.345	0.357	3.046	41.1621	41.162	0.264	0.275	3.035
24	41.1802	41.180	0.345	0.357	3.044	41.1817	41.182	0.264	0.275	3.033
25	41.1976	41.197	0.345	0.357	3.042	41.1989	41.199	0.264	0.275	3.032
26	41.2130	...	0.345		3.041	41.2141	...	0.264		3.031
27	41.2267		0.345		3.039	41.2277		0.264		3.030
28	41.2389		0.345		3.038	41.2398		0.264		3.029
29	41.2499		0.345		3.036	41.2507		0.264		3.028
30	41.2598		0.345		3.035	41.2605		0.264		3.027
31	41.2687		0.345		3.034	41.2694		0.264		3.026
32	41.2768		0.345		3.033	41.2774		0.264		3.025
33	41.2842		0.345		3.032	41.2847		0.264		3.024
34	41.2909		0.345		3.031	41.2914		0.264		3.023
35	41.2970		0.345		3.030	41.2975		0.264		3.023
36	41.3027		0.345		3.029	41.3031		0.264		3.022
37	41.3079		0.345		3.028	41.3083		0.264		3.022
38	41.3126		0.345		3.028	41.3130		0.264		3.021
39	41.3170		0.345		3.027	41.3174		0.264		3.020
40	41.3211		0.345		3.026	41.3214		0.264		3.020
...	...		...		...	...		...		...
∞	41.399	41.399	...	...	3.000	41.399	41.399	...	...	3.000

Table 2. Energy resonances (E_n, eV), quantum defect (δ) and effective nuclear charge Z^* of the Rydberg series due to $4p \rightarrow nd$ transitions from the $^2P°_{1/2}$ metastable state of Rb^{2+} converging to the $4s^24p^4$ ($^1D_2$) series limit in Rb^{3+}

	f_1 ($^2D_2$;$^2P°_{3/2}$) = −0.985 ± 0.080; μ = 8					f_1 ($^2D_2$;$^2P°_{3/2}$) = −0.679 ± 0.080; μ = 8				
	SCUNC	ALS	SCUNC	ALS	SCUNC	SCUNC	ALS	SCUNC	ALS	SCUNC
n	E_n	E_n	δ	δ	Z^*	E_n	E_n	δ	δ	Z^*
8	38.3880	38.388	0.358	0.358	3.141	38.4460	38.446	0.251	0.251	3.097
9	38.8455	38.845	0.358	0.358	3.124	38.8858	38.885	0.250	0.251	3.086
10	39.1685	39.168	0.356	0.358	3.111	39.1974	39.196	0.248	0.251	3.076
11	39.4046	39.403	0.354	0.358	3.100	39.4261	39.425	0.247	0.251	3.069
12	39.5824	39.581	0.353	0.358	3.091	39.5988	39.598	0.245	0.251	3.063
13	39.7196	39.719	0.351	0.358	3.083	39.7324	39.731	0.244	0.251	3.057
14	39.8278	39.827	0.351	0.358	3.077	39.8379	39.837	0.244	0.251	3.053
15	39.9145	39.914	0.350	0.358	3.072	39.9227	39.922	0.243	0.251	3.049
16	39.9851	39.984	0.349	0.358	3.067	39.9919	39.991	0.242	0.251	3.046
17	40.0434	40.043	0.349	0.358	3.063	40.0490	40.048	0.242	0.251	3.043
18	40.0920	40.091	0.348	0.358	3.059	40.0967	40.096	0.241	0.251	3.041
19	40.1330	40.132	0.348	0.358	3.056	40.1370	40.136	0.241	0.251	3.039
20	40.1680	40.167	0.347	0.358	3.053	40.1714	40.171	0.241	0.251	3.037
21	40.1979	40.197	0.347	0.358	3.050	40.2009	40.200	0.241	0.251	3.035
22	40.2238		0.347		3.048	40.2264		0.240		3.033
23	40.2464		0.347		3.046	40.2486		0.240		3.032
24	40.2661		0.347		3.044	40.2681		0.240		3.030
25	40.2835		0.347		3.042	40.2853		0.240		3.029
26	40.2989	...	0.346		3.041	40.3005	...	0.240		3.028
27	40.3126		0.346		3.039	40.3140		0.240		3.027
28	40.3249		0.346		3.038	40.3261		0.240		3.026
29	40.3359		0.346		3.036	40.3370		0.240		3.025
30	40.3457		0.346		3.035	40.3467		0.240		3.024
31	40.3547		0.346		3.034	40.3556		0.240		3.023
32	40.3628		0.346		3.033	40.3636		0.240		3.023
33	40.3702		0.347		3.032	40.3709		0.240		3.022
34	40.3769		0.347		3.031	40.3776		0.240		3.021
35	40.3830		0.347		3.030	40.3837		0.240		3.021
36	40.3887		0.347		3.029	40.3892		0.240		3.020
37	40.3939		0.347		3.028	40.3944		0.240		3.020
38	40.3986		0.347		3.028	40.3991		0.240		3.019
39	40.4030		0.347		3.027	40.4035		0.240		3.019
40	40.4071		0.347		3.026	40.4075		0.240		3.018
...	...		...		...	...		...		...
∞	40.485	40.485	...	...	3.000	40.485	40.485	...	...	3.000

4. Conclusions

The *Screening Constant by Unit Nuclear Charge* (SCUNC) is used to report accurate resonance energies belonging to the $4p \to nd$ transitions from the $^2P°_{3/2}$ ground state and the $^2P°_{1/2}$ metastable state of Rb^{2+} converging to the $4s^24p^4$ ($^1D_2$) series limit in Rb^{3+}. It is seen that the SCUNC formula established reproduces with an excellent precision high-resolution measurements of Macaluso et al. [9]. New data $n = 25$-40 are tabulated as useful guidelines for the NIST data base and for future PI studies on Rb^{2+} focussed on high excited levels.

Competing Interests

The author declares that he has no competing interests.

Authors' Contributions

The author wrote, read and approved the final manuscript.

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