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Single Photoionization Study of Br^{3+} via the Screening Constant by Unit Nuclear Charge Method

Research Article

M. T. Nging and I. Sakho*

Department of Experiential Sciences, UFR Sciences and Technologies, University of Thiès, Thiès, Senegal
***Corresponding author:** aminafatima_sakho@yahoo.fr

Abstract. We report accurate high-lying energy resonances of the Br^{3+} ions. Rydberg series of resonances due to $4p \to nd$ and $4s \to np$ transitions converging respectively to the $4s^24p$ ($^2P_{3/2}$) and $4s4p^2$($^4P_{3/2}$, $^2D_{5/2}$) series limits in Br^{4+} are considered. The calculations are performed using the *screening constant by unit nuclear charge* (SCUNC) method up to $n = 40$. The results obtained are compared with recent ALS measurements of Macaluso *et al.*, [*J. Phys. B: At. Mol. Opt. Phys.* **52** (2019), 145002]. Analysis of the present results is achieved in the framework of the standard quantum-defect theory and of the SCUNC procedure by calculating the effective charge. It is shown that the SCUNC method reproduces excellently the ALS results up to $n = 27$. Our predicted data up to $n = 40$ may be of great importance for the atomic physics community in connection with the modeling of plasma and astrophysical systems.

Keywords. Photoionization; Resonance energies; Rydberg series; Quantum-defect; Effective charge; SCUNC

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1. Introduction

One of the fundamental processes occurring in astrophysical systems is the photoionization of atoms and ions. On the experimental side, merged-beam facilities such as Fourier transform ion cyclotron resonance (FT-ICR) devices at SOLEIL [1] and at Advanced Light Source (ALS)

[2, 3] are largely used in the measurements of accurate photoionization cross sections of atomic systems. For comparison with high-resolution measurements such as those at ALS [2,3], state-of-the-art-theoretical methods are required using highly correlated wave functions, and relativistic effects are required since fine-structure effects can be resolved [4]. Of great important ions interesting to investigate are those of the elements in connection with their abundances in photoionized astrophysical nebulae. For $Z > 30$, neutron (n)-capture elements (e.g., Se, Kr, Br, Xe, Rb, Ba and Pb) produced by slow or rapid n-capture nucleosynthesis [5,6] have been detected in a large number of ionized nebulae [5,7,8]. For the Br^{3+} ion, absolute single photoionization cross-section measurements were performed at ALS and numerous Rydberg series due to the 4p→nd and 4s→np transitions have been identified [15]. As stated by Kim and Mason [10], an important task for the atomic physics community is to provide data for photoionization for modeling of plasma and astrophysical systems. The main motivation of the present work is to provide accurate high-lying energy resonances of Rydberg series of resonances due to 4p→nd and 4s→np transitions that may be useful guidelines for investigators focusing their studies on the photoionization of the Br^{3+} ion. For this purpose, we apply the SCUNC method [11–14,16–18] to provide the first theoretical calculations of the energy resonances of the Rydberg series of resonances due to 4p→nd and 4s→np transitions converging respectively to the $4s^24p$ ($^2P_{3/2}$) and $4s4p^2$($^4P_{3/2}$, $^2D_{5/2}$) series limits in Br^{4+}. Analysis of the present results is achieved in the framework of the standard quantum-defect theory and of the SCUNC procedure by calculating the effective charge. The layout of the present paper is as follows. In Section 2, we present a brief outline of the theoretical part of the work. The presentation and the discussion of the results obtained are given in Section 3 where comparisons are made with the available ALS experimental data [15]. In Section 4 we summarize our study and draw conclusions.

2. Theory

2.1 Brief Description of the SCUNC Formalism

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)

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

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

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

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 (2.1)

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

In this equation, ν and μ ($\mu > \nu$) denote the principal quantum numbers of the ($^{2S+1}L_J$) nlRydberg series used in the empirical determination of the f_i-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. Generally, precise resonance energies are obtained for $q < 5$. The resonance energy are the in the form

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

The quantity $\pm\sum_{k=1}^{q}\sum_{k'=1}^{q'} f_1^{k'} F(n,\mu,\nu,s) \times \left(\frac{1}{Z}\right)^k$ 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 Z_{core} ion, and δ means the quantum defect. In addition, theoretical and measured energy positions can be analyzed by calculating the Z^* effective chargein 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

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

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 Br^{3+} ions, $Z_{\text{core}} = 4$ and $f_2 = (35 - 4) = 31.0$. The remaining f_1-parameter is to be evaluated empirically using the ALS data of Macaluso *et al.*, [15] 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 has been explained in details in our previous works [11–14, 16–18].

2.2 Resonance Energies of the 4p→*n*d and 4s→*n*p Transitions

Using eq. (2.5), we obtain the following energy positions (in Rydberg)

- For the Rydberg series of resonances due to 4p→nd transitions from the $^1D_2$ excited states of Br^{3+} converging to the $^2P_{3/2}$series limit in Br^{4+}

$$E_n = E_\infty - \frac{Z^2}{n^2}\left\{1 - \frac{f_1(^1D_2)}{Z(n-1)} - \frac{f_2(^1D_2)}{Z} - \frac{f_1(^1D_2)\times(n-\mu)}{Z^2(n+\mu+s-1)\times(n+\mu-s)}\right\}^2. \tag{2.12}$$

- For the Rydberg series of resonances due to 4p→nd transitions from the $^3P_2$ excited states of Br^{3+} converging to the $^2P_{3/2}$ series limit in Br^{4+}

$$E_n = E_\infty - \frac{Z^2}{n^2}\left\{1 - \frac{f_1(^3P_2)}{Z(n-1)} - \frac{f_2(^3P_2)}{Z} - \frac{f_1(^3P_2)\times(n-\mu)}{Z^2(n+\mu+s-1)\times(n+\mu-s+1)}\right\}^2. \tag{2.13}$$

- For the Rydberg series of resonances due to 4p→nd transitions from the $^3P_1$ excited states of Br^{3+} converging to the $^2P_{3/2}$ series limit in Br^{4+}

$$E_n = E_\infty - \frac{Z^2}{n^2}\left\{1 - \frac{f_1(^3P_1)}{Z(n-1)} - \frac{f_2(^3P_1)}{Z} - \frac{f_1(^3P_1)\times(n-\mu)}{Z^2(n+\mu+s-1)\times(n+\mu-s+1)} - \frac{f_1(^3P_1)\times(n-\mu)}{Z^3(n+\mu+s)\times(n+\mu-s+1)}\right\}^2. \tag{2.14}$$

- For the Rydberg series of resonances due to 4s→np transitions from the $^3P_1$ states of Br^{3+} converging to the $^4P_{3/2}$series limit in Br^{4+}

$$E_n = E_\infty - \frac{Z^2}{n^2}\left\{1 - \frac{f_1(^3P_1)}{Z(n-1)} - \frac{f_2(^3P_1)}{Z} - \frac{f_1(^3P_1)\times(n-\mu-1)\times(n-\mu)}{Z^2(n+\mu+2s-1)^2}\right\}^2. \tag{2.15}$$

- For the Rydberg series of resonances due to 4s→np transitions from the $^1D_2$ states of Br^{3+} converging to the $^2D_{5/2}$ series limit in Br^{4+}

$$E_n = E_\infty - \frac{Z^2}{n^2}\left\{1 - \frac{f_1(^1D_2)}{Z(n-1)} - \frac{f_2(^1D_2)}{Z} - \frac{f_1(^1D_2)\times(n-\mu-1)\times(n-\mu)}{Z^2(n+\mu+s+3)^2}\right\}^2. \tag{2.16}$$

3. Results and Discussion

Let us first precise the sign of the quantum defect δ using the SCUNC analysis conditions (2.9) by considering the lowest resonance corresponding to the first entry for the Rydberg series investigated. For this purpose, we focus the demonstration on the particular case of the Rydberg series of resonances due to 4p→nd transitions from the $^1D_2$ excited states of Br^{3+}

converging to the $^2P_{3/2}$ series limit in Br^{4+}. The calculations are of similar for the other series. The lowest resonance corresponds to the 4p→18d transition ($\mu_{low} = 18$). From Table 1, we pull $f_1(^1D_2) = -3.6035$. From Eq. (2.10), we deduce the expression of the effective charge Z^*_{max} as follows

$$Z^*_{max} = Z_0 \left\{ 1 - \frac{f_1\left(^1D_2\right)}{Z_0\left(\mu_{low} - 1\right)} - \frac{31.0}{Z_0} \right\} = 37 \left\{ 1 - \frac{3.6035}{35(18-1)} - \frac{31.0}{35} \right\} = 4.212. \tag{3.1}$$

As $Z_{core} = 4.0$, so $Z^*_{max} = 4.212 > Z_{core}$. The quantum defect δ is then positive according to the SCUNC analysis conditions (2.9). Let us now move on comparing the present predictions for the resonance energies with available literature data. The data are quoted in Tables 1–5.

In Table 1 we quote the present SCUNC results for energy resonances (E), quantum defects (δ) and effective charge (Z^*) of the series due to 4p→nd transitions from the $^1D_2$ excited states of Br^{3+} converging to the $^2P_{3/2}$ series limit in Br^{4+}. It is seen that the data obtained compared very well with the experimental data of Macaluso *et al.*, [15]. Up to n = 27, the energy differences relative to the experimental data is 0.000 eV which proves that the SCUNC method perfectly reproduces the experimental results. In Tables 2 and 3 the present SCUNC data for energy resonances (E), quantum defects (δ) and effective charge (Z^*) respectively for the Rydberg series due to the 4p→nd transitions from the $^3P_2$ and from the $^3P_1$ excited states of Br^{3+} converging to the $^2P_{3/2}$ series limit in Br^{4+} are listed. Comparison indicates excellent agreements with the ALS measurements [15]. In Table 3, the energy differences have never overrun 0.001 eV. In Table 4 and 5 are presented the SCUNC predictions for energy resonances (E), quantum defects (δ) and effective charge (Z^*) of the Rydberg series of resonances due to 4s→np transitions from the $^1D_2$ states of Br^{3+} converging to the $^4P_{3/2}$ series limit in Br^{4+} to the experimental data [15]. Except for n = 7 and 8, the maximum energy differences relative to the experimental data is at 0.009 eV up to n = 17İn Table 5, we list the present results for resonances due to 4s→np transitions from the $^3P_1$ states of Br^{3+} converging to the $^2D_{5/2}$ series limit in Br^{4+} to the experimental data [15]. Here again, good agreements with the ALS data [15] are obtained. The slight discrepancies between the present calculations and the ALS measurements [15] may be explained by the simplicity of the SCUNC formalism which does not include explicitly any relativistic corrections. In addition, for all the Rydberg series investigated, the quantum defects obtained via the SCUNC formalism are almost constant along all the series up to $n = 40$. The effective charges are also seen to tend toward $Z_{core} = 4.0$ with increasing n as predicted by the SCUNC analysis procedure (2.9).

4. Summary and Conclusion

The first calculations of resonance energies and quantum defects of the Rydberg series of resonances due to 4p→nd and 4s→np transitions converging respectively to the $4s^24p$ ($^2P_{3/2}$) and $4s4p^2$($^4P_{3/2}$, $^2D_{5/2}$) series limits in Br^{4+} have been investigated. Calculations are performed in the framework of the *Screening Constant by Unit Nuclear Charge* (SCUNC) method up to $n = 40$. Excellent agreements are obtained between the present predictions and very recent Advanced Light Source experiments of Macaluso *et al.*, [15] at Lawrence Berkeley

National Laboratory. The very good results obtained in this work show that the SCUNC-method can be used to assist the sophisticated R-matrix-method for locating and determining the properties of atomic resonances. New high lying accurate resonance energies are tabulated as benchmarked data for interpreting Br^{3+} spectra from nebulae. These high lying Rydberg series tabulated may also be very useful data for the NIST database.

Table 1. Energy resonances (E), quantum defect (δ) and effective charge (Z^*) of the series of resonances due to 4p→nd transitions from the $^1D_2$ excited states of Br^{3+} converging to the $^2P_{3/2}$ series limit in Br^{4+}. $f_1(^1D_2) = -3.6035$; $\mu = 18$. The present results (SCUNC) are compared with the experimental data from ALS measurements of Macaluso *et al.*, [15]. $|\Delta E|$ denotes the energy difference between the SCUNC calculations and the ALS measurements

Initial Br^{3+} state $4s^24p^2(^1D_2)$						
$4s^24p(^1D_2)nd$ Rydberg series						
	Theory			Experiment		
	SCUNC			ALS		
n	E (eV)	δ	Z^*	E (eV)	δ	$\|\Delta E\|$
18	44.995	0.906	4.212	44.995	0.902	0.000
19	45.075	0.906	4.200	45.075	0.902	0.000
20	45.143	0.906	4.190	45.143	0.902	0.000
21	45.201	0.906	4.180	45.201	0.902	0.000
22	45.251	0.906	4.172	45.251	0.902	0.000
23	45.294	0.906	4.164	45.294	0.902	0.000
24	45.332	0.906	4.157	45.332	0.902	0.000
25	45.365	0.906	4.150	45.365	0.902	0.000
26	45.394	0.907	4.144	45.394	0.902	0.000
27	45.420	0.907	4.139	45.420	0.902	0.000
28	45.443	0.907	4.133			
29	45.464	0.907	4.129			
30	45.483	0.907	4.124			
31	45.500	0.907	4.120			
32	45.515	0.908	4.116			
33	45.529	0.908	4.113			
34	45.541	0.908	4.109			
35	45.553	0.908	4.106			
36	45.563	0.908	4.103			
37	45.573	0.909	4.100			
38	45.582	0.909	4.097			
39	45.590	0.909	4.095			
40	45.598	0.909	4.092			
...	...		...			
∞	45.740		4.000	45.740		

Table 2. Energy resonances (E), quantum defect (δ) and effective charge (Z^*) of the series of resonances due to $4p \rightarrow nd$ transitions from the $^3P_2$ excited states of Br^{3+} converging to the $^2P_{3/2}$ series limit in Br^{4+}. $f_1(^3P_2) = -3.7475$; $\mu = 18$. The present results (SCUNC) are compared with the experimental data from ALS measurements of Macaluso *et al.*, [15]. $|\Delta E|$ denotes the energy difference between the SCUNC calculations and the ALS measurements

Initial Br^{3+} state $4s^2 4p^2 (^3P_2)$						
	$4s^2 4p(^3P_2)nd$ Rydberg series					
	Theory			Experiment		
	SCUNC			ALS		
n	E (eV)	δ	Z^*	E (eV)	δ	$\|\Delta E\|$
18	46.303	0.940	4.220	46.303	0.948	0.000
19	46.384	0.940	4.208	46.383	0.948	0.001
20	46.452	0.940	4.197	46.451	0.948	0.001
21	46.510	0.940	4.187	46.510	0.948	0.000
22	46.560	0.941	4.178	46.560	0.948	0.000
23	46.604	0.941	4.170	46.604	0.948	0.000
24	46.642	0.941	4.163	46.642	0.948	0.000
25	46.675	0.941	4.156	46.675	0.948	0.000
26	46.704	0.941	4.150	46.704	0.948	0.000
27	46.730	0.942	4.144	46.730	0.948	0.000
28	46.754	0.942	4.139			
29	46.774	0.942	4.134			
30	46.793	0.942	4.129			
31	46.810	0.943	4.125			
32	46.825	0.943	4.121			
33	46.839	0.943	4.117			
34	46.852	0.943	4.114			
35	46.863	0.943	4.110			
36	46.874	0.944	4.107			
37	46.884	0.944	4.104			
38	46.892	0.944	4.101			
39	46.901	0.944	4.099			
40	46.908	0.945	4.096			
...	...		...			
∞	47.051		4.000	47.051		

Table 3. Energy resonances (E), quantum defect (δ) and effective charge (Z^*) of the series of resonances due to 4p→nd transitions from the $^3P_1$ excited states of Br^{3+} converging to the $^2P_{3/2}$ series limit in Br^{4+}. $f_1(^3P_1) = -3.6995$; $\mu = 18$. The present results (SCUNC) are compared with the experimental data from ALS measurements of Macaluso *et al.*, [15]. $|\Delta E|$ denotes the energy difference between the SCUNC calculations and the ALS measurements

Initial Br^{3+} state $4s^24p^2(^3P_1)$						
$4s^24p(^3P_1)nd$ Rydberg series						
	Theory			Experiment		
	SCUNC			ALS		
n	E (eV)	δ	Z^*	E (eV)	δ	$\|\Delta E\|$
18	46.675	0.928	4.218	46.675	0.928	0.000
19	46.755	0.929	4.206	46.755	0.928	0.000
20	46.823	0.929	4.195	46.823	0.928	0.000
21	46.882	0.929	4.185	46.882	0.928	0.000
22	46.932	0.929	4.176	46.932	0.928	0.000
23	46.975	0.929	4.168			
24	47.013	0.929	4.161			
25	47.046	0.930	4.154			
26	47.076	0.930	4.148			
27	47.102	0.930	4.142			
28	47.125	0.930	4.137			
29	47.146	0.930	4.132			
30	47.164	0.931	4.128			
31	47.181	0.931	4.123			
32	47.196	0.931	4.119			
33	47.210	0.931	4.116			
34	47.223	0.932	4.112			
35	47.234	0.932	4.109			
36	47.245	0.932	4.106			
37	47.255	0.932	4.103			
38	47.264	0.932	4.100			
39	47.272	0.933	4.097			
40	47.279	0.933	4.095			
...	...		...			
∞	47.422		4.000	47.422		

Table 4. Energy resonances (E), quantum defect (δ) and effective charge (Z^*) of the Rydberg series of resonances due to 4s→np transitions from the $^3P_1$ states of Br^{3+} converging to the $^4P_{3/2}$ series limit in Br^{4+}. $f_1(^3P_1) = -2.31904$; $\mu = 5$. The present results (SCUNC) are compared with the experimental data from ALS measurements of Macaluso *et al.*, [15]. $|\Delta E|$ denotes the energy difference between the SCUNC calculations and the ALS measurements

Initial Br^{3+} state $4s^24p^2(^3P_1)$						
$4s4p^2(^3P_1)np$ Rydberg series						
	Theory			Experiment		
	SCUNC			ALS		
n	E (eV)	δ	Z^*	E (eV)	δ	$\|\Delta E\|$
5	47.190	0.633	4.580	47.190	0.633	0.000
6	51.071	0.625	4.464	51.047	0.633	0.000
7	53.255	0.621	4.387	53.235	0.633	0.020
8	54.608	0.620	4.331	54.594	0.633	0.014
9	55.504	0.621	4.290	55.495	0.633	0.009
10	56.128	0.625	4.258	56.124	0.633	0.004
11	56.581	0.629	4.232	56.579	0.633	0.002
12	56.919	0.635	4.211	56.920	0.633	0.001
13	57.179	0.643	4.193	57.182	0.633	0.003
14	57.383	0.650	4.178	57.387	0.633	0.004
15	57.546	0.659	4.166	57.550	0.633	0.004
16	57.679	0.669	4.155	57.683	0.633	0.004
17	57.788	0.679	4.145	57.792	0.633	0.004
18	57.879	0.689	4.136			
19	57.955	0.700	4.129			
20	58.020	0.711	4.122			
21	58.076	0.723	4.116			
22	58.124	0.735	4.110			
23	58.165	0.747	4.105			
24	58.202	0.760	4.101			
25	58.234	0.773	4.097			
26	58.263	0.786	4.093			
27	58.288	0.799	4.089			
28	58.310	0.812	4.086			
29	58.331	0.826	4.083			
30	58.349	0.839	4.080			
31	58.365	0.853	4.077			
32	58.380	0.867	4.075			
33	58.394	0.881	4.072			
34	58.406	0.895	4.070			
35	58.418	0.910	4.068			
36	58.428	0.924	4.066			
37	58.438	0.938	4.064			
38	58.446	0.953	4.063			
39	58.454	0.967	4.061			
40	58.462	0.982	4.059			
...	...		...			
∞	58.605		4.000	58.605		

Table 5. Energy resonances (E), quantum defect (δ) and effective charge (Z^*) of the Rydberg series of resonances due to $4s \to np$ transitions from the $^1D_2$ states of Br^{3+} converging to the $^2D_{5/2}$ series limit in Br^{4+}. $f_1(^1D_2) = -2.41188$; $\mu = 5$. The present results (SCUNC) are compared with the experimental data from ALS measurements of Macaluso *et al.*, [15]. $|\Delta E|$ denotes the energy difference between the SCUNC calculations and the ALS measurements

Initial Br^{3+} state $4s^24p^2(^1D_2)$						
$4s4p^2(^1D_2)np$ Rydberg series						
	Theory			Experiment		
	SCUNC			ALS		
n	E (eV)	δ	Z^*	E (eV)	δ	$\|\Delta E\|$
5	48.784	0.655	4.603	48.784	0.655	0.000
6	52.719	0.646	4.482	52.695	0.655	0.024
7	54.930	0.642	4.402	54.907	0.655	0.023
8	56.297	0.640	4.345	56.280	0.655	0.017
9	57.200	0.640	4.301	57.189	0.655	0.011
10	57.830	0.641	4.268	57.822	0.655	0.008
11	58.285	0.644	4.241	58.281	0.655	0.004
12	58.626	0.648	4.219	58.623	0.655	0.003
13	58.887	0.654	4.201	58.886	0.655	0.001
14	59.092	0.660	4.186	59.092	0.655	0.000
15	59.255	0.667	4.172	59.257	0.655	0.002
16	59.388	0.674	4.161	59.390	0.655	0.002
17	59.497	0.682	4.151	59.500	0.655	0.003
18	59.588	0.691	4.142			
19	59.665	0.701	4.134			
20	59.730	0.710	4.127			
21	59.786	0.721	4.121			
22	59.834	0.731	4.115			
23	59.876	0.742	4.110			
24	59.912	0.754	4.105			
25	59.944	0.765	4.100			
26	59.973	0.777	4.096			
27	59.998	0.789	4.093			
28	60.021	0.802	4.089			
29	60.041	0.814	4.086			
30	60.059	0.827	4.083			
31	60.076	0.840	4.080			
32	60.091	0.853	4.078			
33	60.104	0.866	4.075			
34	60.117	0.880	4.073			
35	60.128	0.894	4.071			
36	60.138	0.907	4.069			
37	60.148	0.921	4.067			
38	60.157	0.935	4.065			
39	60.165	0.950	4.063			
40	60.172	0.964	4.062			
...	...		...			
∞	60.315		4.000	60.315		

Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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