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

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Abstract. We report accurate high-lying energy resonances of the Br$^{3+}$ ions. Rydberg series of resonances due to $4p\rightarrow nd$ and $4s\rightarrow np$ 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)
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[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 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$^2$4p ($^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)

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

(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

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

(2.2)

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

For a given Rydberg series originating from a $^{2S+1}L_J$ state, we obtain using (2.1)

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

(2.3)
In this equation, \( \nu \) and \( \mu \) \((\mu > \nu)\) denote the principal quantum numbers of the \( (2S+1L_J) \) \( nl \) Rydberg series used in the empirical determination of the \( f_i \)-screening constants, \( s \) represents the spin of the \( nl \)-electron \((s = \frac{1}{2})\), \( E_\infty \) is the energy value of the series limit, \( E_n \) denotes the resonance energy and \( Z \) stands for the atomic number. The \( \beta \)-parameters are screening constants by unit nuclear charge expanded in inverse powers of \( Z \) and given by

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

where \( f_k = f_k(2S+1L_J, n, s, \mu, \nu) \) are screening constants to be evaluated empirically.

In eq. \((2.2)\), \( q \) stands for the number of terms in the expansion of the \( \beta \)-parameter. Generally, precise resonance energies are obtained for \( q < 5 \). The resonance energy are the in the form

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

The quantity \( \pm \sum_{k=1}^{q} \sum_{k'=1}^{q'} f_k' F(n, \mu, \nu, s) \times \left( \frac{1}{Z} \right)^k \) 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

\[
E_n = E_\infty - \frac{RZ^2}{(n-\delta)^2}.
\]  

In this equation, \( R \) is the Rydberg constant, \( E_\infty \) denotes the converging limit, \( Z_{\text{core}} \) represents the electric charge of the \( Z_{\text{core}} \) ion, and \( \delta \) 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

\[
E_n = E_\infty - \frac{Z^2}{n^2} R.
\]  

The relationship between \( Z^* \) and \( \delta \) is in the form

\[
Z^* = \frac{Z_{\text{core}}}{(1 - \frac{\delta}{n})}.
\]  

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

\[
\begin{align*}
Z^* &\geq Z_{\text{core}} \quad \text{if } \delta \geq 0 \\
Z^* &\leq Z_{\text{core}} \quad \text{if } \delta \leq 0 \\
\lim_{n \to \infty} Z^* &\approx Z_{\text{core}}
\end{align*}
\]  

Besides, comparing Eq. \((2.3)\) and Eq. \((2.7)\), the effective charge is in the form

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

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

\[
\lim_{n \to \infty} Z^* = Z \left( 1 - \frac{f_2(2S+1L)}{Z} \right) = Z_{\text{core}}.
\]
We get then $f_2 = Z - Z_{\text{core}}$, where $Z_{\text{core}}$ is directly obtained by the photoionization process from an atomic $X^p+$ system $X^p+ + h\nu \rightarrow X^{(p+1)+} + e^-$. 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. for a given $(2^S + 1)L_J$ $\mu l$ 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.

2.2 Resonance Energies of the 4p$\rightarrow$nd and 4s$\rightarrow$np Transitions

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

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

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

- For the Rydberg series of resonances due to 4s$\rightarrow$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$\rightarrow$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 $\delta$ 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$\rightarrow$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 ($\mu_{\text{low}} = 18$). From Table I, we pull $f_1(\mu_{D_2}) = -3.6035$. From Eq. (2.14), we deduce the expression of the effective charge $Z_{\text{max}}^*$ as follows

$$Z_{\text{max}}^* = Z_0 \left\{ 1 - \frac{f_1(\mu_{D_2})}{Z_0(\mu_{\text{low}} - 1)} \right\} = 37 \left\{ 1 - \frac{3.6035}{35(18 - 1)} \right\} = 4.212. \quad (3.1)$$

As $Z_{\text{core}} = 4.0$, so $Z_{\text{max}}^* = 4.212 > Z_{\text{core}}$. The quantum defect $\delta$ 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 II–IV.

In Table II we quote the present SCUNC results for energy resonances ($E$), quantum defects ($\delta$) 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 II and III the present SCUNC data for energy resonances ($E$), quantum defects ($\delta$) 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 III, the energy differences have never overrun 0.001 eV. In Table IV and V are presented the SCUNC predictions for energy resonances ($E$), quantum defects ($\delta$) 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 $n = 17$. In Table V, 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 $Z_{\text{core}} = 4.0$ 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$^2$4p ($^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

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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 ($\delta$) and effective charge ($Z^*$) of the series of resonances due to 4p$\rightarrow$n$d$ 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.

| $n$ | $E$ (eV) | $\delta$ | $Z^*$ | $E$ (eV) | $\delta$ | $|\Delta E|$ |
|----|--------|------|-----|--------|------|--------|
| 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 |          |      |        |
| ... | ... | ... | ... |          |      |        |
| \(\infty\) | 45.740 | 4.000 | \(45.740\) |
Table 2. Energy resonances ($E$), quantum defect ($\delta$) and effective charge ($Z^*$) of the series of resonances due to $4p-n\text{d}$ transitions from the $^3P_2$ excited states of $\text{Br}^{3+}$ converging to the $^2P_{3/2}$ series limit in $\text{Br}^{4+}$. $f_1(^3P_2) = -3.7475$; $\mu = 18$. The present results (SCUNC) are compared with the experimental data from ALS measurements of Macaluso et al. |$\Delta E$| denotes the energy difference between the SCUNC calculations and the ALS measurements.

| $n$ | $E$ (eV) | $\delta$ | $Z^*$ | $E$ (eV) | $\delta$ | $|\Delta E|$ |
|-----|---------|--------|------|---------|--------|-------------|
| 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| 46.754  | 0.942  | 0.000       |
| 29  | 46.774  | 0.942  | 4.134| 46.774  | 0.942  | 0.000       |
| 30  | 46.793  | 0.942  | 4.129| 46.793  | 0.942  | 0.000       |
| 31  | 46.810  | 0.943  | 4.125| 46.810  | 0.943  | 0.000       |
| 32  | 46.825  | 0.943  | 4.121| 46.825  | 0.943  | 0.000       |
| 33  | 46.839  | 0.943  | 4.117| 46.839  | 0.943  | 0.000       |
| 34  | 46.852  | 0.943  | 4.114| 46.852  | 0.943  | 0.000       |
| 35  | 46.863  | 0.943  | 4.110| 46.863  | 0.943  | 0.000       |
| 36  | 46.874  | 0.944  | 4.107| 46.874  | 0.944  | 0.000       |
| 37  | 46.884  | 0.944  | 4.104| 46.884  | 0.944  | 0.000       |
| 38  | 46.892  | 0.944  | 4.101| 46.892  | 0.944  | 0.000       |
| 39  | 46.901  | 0.944  | 4.099| 46.901  | 0.944  | 0.000       |
| 40  | 46.908  | 0.945  | 4.096| 46.908  | 0.945  | 0.000       |
| ... | ...     | ...    | ...  | ...     | ...    | ...         |
| $\infty$ | 47.051  | 4.000  | 47.051|                   |        |              |
Table 3. Energy resonances ($E$), quantum defect ($\delta$) and effective charge ($Z^*$) of the series of resonances due to $4p-n_d$ 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.

| $n$ | SCUNC | ALS | Experiment |
|-----|--------|-----|------------|
|     | $E$ (eV) | $\delta$ | $Z^*$ | $E$ (eV) | $\delta$ | $|\Delta E|$ |
| 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 |          |       |       |
| ... | ...     | ...  | ...   |          |       |       |
| $\infty$ | 47.422  | 4.000 | 47.422 |          |       |       |
Table 4. Energy resonances ($E$), quantum defect ($\delta$) 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.

| n  | $E$ (eV) | $\delta$ | $Z^*$ | $E$ (eV) | $\delta$ | $|\Delta E|$ |
|---|--------|--------|------|--------|--------|--------|
| 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 |        |        |        |
| ... | ... | ... | ... |        |        |        |
| \(\infty\) | 58.605 | 4.000 | 58.605 |        |        |        |
Table 5. Energy resonances ($E$), quantum defect ($\delta$) 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 $^2D_{5/2}$ 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.

| $n$ | Theory | Experiment |
|-----|--------|------------|
|     | SCUNC  | ALS        |
|     | $E$ (eV) $\delta$ $Z^*$ | $E$ (eV) $\delta$ $|\Delta E|$ |
| 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 |           |
| ... | ...    | ...        |
| $\infty$ | 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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