K-shell Photoionization of Be-like nitrogen from the ground state
: Energies and Auger widths of the high-lying double-excited states for N IV

<table>
<thead>
<tr>
<th>Journal:</th>
<th>Canadian Journal of Physics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Manuscript ID</td>
<td>cjp-2017-0601.R3</td>
</tr>
<tr>
<td>Manuscript Type:</td>
<td>Article</td>
</tr>
<tr>
<td>Date Submitted by the Author:</td>
<td>13-Jan-2018</td>
</tr>
<tr>
<td>Complete List of Authors:</td>
<td>Liang, Liang; Department of Physics, Xi'an University of Architecture and Technology Zhou, Chao; Xi'an University of Architecture and Technology, Physics department</td>
</tr>
<tr>
<td>Keyword:</td>
<td>photoionization, R-matrix, QB method, autoionizing energy levels, doubly-excited state</td>
</tr>
<tr>
<td>Is the invited manuscript for consideration in a Special Issue?:</td>
<td>N/A</td>
</tr>
</tbody>
</table>

https://mc06.manuscriptcentral.com/cjp-pubs
K-shell Photoionization of Be-like nitrogen from the ground state: Energies and Auger widths of the high-lying double-excited states for N IV

Liang Liang*, Chao Zhou

Physics department, Xi’an University of Architecture and Technology, Xi’an 710055, People’s Republic of China

Abstract:
The K-shell photoionization (PI) cross section of Be-like nitrogen (N IV) from the ground state is studied with the R-matrix and distorted-wave method for photon energies from 5.7 to 41.2 Ry. The close-coupling expansion includes thirty-four target states of N V with the thirteen configurations in the LS-coupling scheme. The resonance energies, quantum defect and widths of eighteen series of autoionization are determined from QB method and agree with these by cross sections. Our theoretical resonance energies, widths are compared with the existing experiments on the Auger spectra and other theoretical results. The results show that the calculated resonance energies are in rather good agreement with the experiment on the Auger spectra. For the autoionization width of some resonance states, good agreement is also found with recent theoretical results wherever available obtained using a saddle-point complex-rotation method.

PACS number(s): 32.80.Fb

Key words: photoionization; R-matrix; QB method; autoionizing energy levels; doubly-excited state.

1. Introduction

Photoionization (PI) cross sections are very important in many fields, such as astrophysical modelings for opacities, modelling of laboratory, astrophysical plasmas, fusion plasmas, spectral analysis, ionization balance, recombination cascade matrix, etc. On the other hand, the studies of the Auger spectra of the doubly-excited states play an important role in understanding the collision mechanism and atomic structure, and are also helpful in plasmas diagnostics.

Due to the photoionization of the Be-like ions offers an opportunity to study electron correlation of the simplest multishell atom and ions, a large number of studies such as PI cross sections, energies and widths of doubly-excited states and oscillator strengths for the beryllium isoelectronic sequence have been made in the past few decades[1-8].

For example, in the 1990s, Berrington et al. [9] had studied the PI cross section of Be isoelectronic sequence using R-matrix and obtained a rough figure of PI cross section for N IV. Subsequently, the autoionization of the states of manifolds 1s23l3l' and 1s33l4l in N3+ were studied experimentally and theoretically by Kitazaway et al. [11]. In addition, basing on the Breit–Pauli R-matrix method Garcia et al. [10] investigated the high-energy photoabsorption cross sections for nitrogen ions in the K-edge region, and obtained the K-vacancy level energies, wavelengths, Einstein A-coefficients, radiative and Auger widths of N IV. Recently, Li et al. [12] have studied the relativistic energies, radiative and Auger rates of the high-lying doubly-excited 1s23l3l' 1,3L states of the Be.

* E-mail: liangll501@sina.com
isoelectronic sequence using the saddle-point variational method with complex rotation. Hsin et al. [13] have calculated the energy and width for the single core-excited Be-like $1s2s^22p \, ^1P^o$, $1s2p^3 \, ^1P^o$, and $1s2s^23p \, ^1P^o$. Furthermore, Auger resonances $1s2s^2 \, 2p \, ^1S^o$ has been studied by Song et al. [4] by means of the complex-scaled multireference configuration interaction method. However, to our knowledge, there is not any detailed study on the photoionization cross sections of N IV.

In the present work, basing on the $R$-matrix, QB and Breit-Pauli relativistic distorted-wave methods, we have calculated the K-shell photoionization cross-sections (length gauges) from the ground state, resonance energies and widths for eighteen Rydberg series of N IV.

2. Theory

The R-matrix approach [16-18] is a highly sophisticated and useful method in atomic physics. The basic atomic theory relevant to the $R$-matrix approximation was given in Refs. [15,18] and the detailed description of the computer codes was given in Ref. [17]. Here we only present a brief outline of the theory relevant to the calculation of photoionization cross sections.

The $(N+1)$-electron wavefunction in the internal region is given by Ref. [18] as follows:

$$
\psi_i(x_1,x_2,\ldots,x_{N+1}) = A \sum_j c_{ijk} \Phi_j(x_1,x_2,\ldots,x_{N+1}; \hat{r}_{N+1}\sigma_{N+1}) \frac{1}{r_{N+1}} u_j(r_{N+1}) + \sum_j d_{jk} \chi_j(x_1,x_2,\ldots,x_{N+1})
$$

(1)

where $\Phi_j$ are the target state wavefunctions coupled with the angular and spin parts of the photoelectron, and $A$ is the antisymmetry operator. The $u_j$ and $\chi_j$ represent the continuum wavefunctions and the $(N+1)$-electron bound state wavefunctions of photoelectron, respectively. The wavefunction in the external region is given as follows:

$$
\psi_k = \sum_j c_{ijk} \Phi_j(x_1,x_2,\ldots,x_{N+1}; \hat{r}_{N+1}\sigma_{N+1}) \frac{1}{r_{N+1}} u_j(r_{N+1})
$$

(2)

The parameters $c_{ijk}$ and $d_{jk}$ may be calculated by diagonalizing the $(N+1)$-electron Hamiltonian within the inner region of the $R$-matrix box. By enforcing continuity at the boundary, then we can get the wavefunctions in both regions with the $R$-matrix as a connection between the parts.

The total PI cross section in atomic unit is given by

$$
\sigma_{pl} = \frac{4\pi^2 a_0^2 \alpha}{3} \frac{\omega}{g_j} S.
$$

(3)

Here $\alpha$ is the fine-structure constant $e^2/\hbar c$, $a_0$ is the Bohr radius, $g_j$ is the statistical weight of the initial bound state $j$, and the $\omega$ is the incident photon energy in Ry. Noting that the line strength $S$ corresponds to a transition from an initial $(N+1)$-electron bound state $j$ of energy $E_j$ to the final continuum states of energy $\epsilon = E_j + \omega$. Moreover, the generalized line strength is obtained from dipole transition $(E_j \rightarrow \epsilon)$ matrix elements by

$$
S(\epsilon,j) = \sum_{l_j,j_\epsilon} \left| <l_j,J_j,\epsilon D||j>|^2,
$$

(4)

where the summation runs over all the continuum states that are dipole allowed with respect to the initial state $j$.

The QB method [14] is adopted in this work to determine the resonance energies and widths. The QB method works in the $R$-matrix environment, and the reactance matrix $K$ is computed by
matching the inner-region radial functions to $n \times n_o$ linear combinations of the outer-region radial functions for $n_o$ open channels, where the $n$ is the total number of channels retained in the close-coupling expansion. The $K_{oo}$ may be obtained by diagonalizing the $K$ matrix in open-channel space, and the eigenphase for each channel may be calculated by using the eigenvalues $\lambda_i$.

$$\delta_i = \tan^{-1} \lambda_i, \quad i = 1, 2, \ldots, n_o.$$  \hspace{1cm} (5)

The sum over all channels gives the eigenphase sum $\delta$ which represents the resonance behavior of PI cross section. The resonance position is computed by the energy of the maximum gradient $d\delta/dE = \delta'$, and the resonance widths at the resonance energy $E_r$ is given in Ref.[14] as below:

$$\Gamma = 2 / \delta'(E_r).$$  \hspace{1cm} (6)

3. Results and discussion

In order to analyze evidently the resonance structures, we employ the LS-coupling form. For the beryllium-like N IV, the thirteen lowest LS-coupling target states of ion N V are used. In the present investigation we considered the photon energy region from 5.69 Ry to 41.2Ry.

The photoionization process is shown as follow:

$$h\nu + N^{+\ast}(1s^2 2s^2 1S) \rightarrow N^+1s^2 2s(1S) + e^-(kp) 1P$$

$$\rightarrow N^+1s^2 2p(1P) + e^-(ks, kd) 1P$$

$$\rightarrow N^+1s^2 3s(1S) + e^-(kp) 1P$$

$$\rightarrow N^+1s^2 3p(1P) + e^-(ks, kd) 1P$$

$$\rightarrow N^+1s^2 3d(1D) + e^-(kp, kf) 1P$$

$$\rightarrow N^+1s^2 4s(1S) + e^-(kp, kf) 1P$$

$$\rightarrow N^+1s^2 4p(1P) + e^-(ks, kd) 1P$$

$$\rightarrow N^+1s^2 4s(1S) + e^-(kp, kf) 1P$$

In order to obtain the orbital wave-function of the target ion N V for $R$-matrix, the AUTOSTRUCTURE (AS) [15] of distorted-wave method is employed, and the total ten orbital wave-functions $1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d$ and $4f$ of N V are calculated by using and optimizing the thirty-four energy states of the thirteen configurations for N V $1s^2nl (n=2-4$ and $l=0-3), 1s^22p^2, 1s2s2p, 1s2p^2$ and $1s2s3s$. These calculated target state energies are listed in Table 1. From Table 1, we can see that our results are excellently well in accordance with the existing experiments and theoretical results. Simultaneously, the calculated results also show that the obtained orbits wave-functions are reasonable.

The radius of $R$-matrix box is chosen to be 14.34113 a.u. to contain all bound orbitals, where 30 continuum orbitals for each channel are included. In order to ensure that all the resonance structures are properly delineated in PI cross sections, we adopted the 50000 energy mesh points, and the energy increment is 0.000001 Ry in the calculations. Though the calculated energies listed in Table 1 using the $R$-matrix method are close to measured values, in order to ensure the accuracy of the calculated PI cross section, we have used the experimental values of excitation energies of the target ion ($1s^2 2s^2 S, 1s^2 2p^2 P, 1s^2 3s^2 S, 1s^2 3p^2 P$ and $1s^2 3d^2 D$) in our calculations.

Table 1. The energies levels (Ry) of target ion N V

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$1s^22s^2S$</td>
<td>0.00000</td>
<td>0.00000</td>
</tr>
<tr>
<td>$n$</td>
<td>$E_r$ (Ry)</td>
<td>$\mu$</td>
<td>NIST[20]</td>
</tr>
<tr>
<td>-----</td>
<td>-------------</td>
<td>-------</td>
<td>----------</td>
</tr>
<tr>
<td>5</td>
<td>5.72038</td>
<td>0.2483</td>
<td>5.72774</td>
</tr>
<tr>
<td>6</td>
<td>5.94535</td>
<td>0.2483</td>
<td>6.14903</td>
</tr>
<tr>
<td>7</td>
<td>6.07802</td>
<td>0.2482</td>
<td>3.7333E-03</td>
</tr>
<tr>
<td>8</td>
<td>6.16274</td>
<td>0.2482</td>
<td>2.4133E-03</td>
</tr>
<tr>
<td>9</td>
<td>6.22012</td>
<td>0.2480</td>
<td>1.6223E-03</td>
</tr>
<tr>
<td>10</td>
<td>6.26076</td>
<td>0.2481</td>
<td>1.1603E-03</td>
</tr>
<tr>
<td>11</td>
<td>6.29060</td>
<td>0.2482</td>
<td>8.601E-04</td>
</tr>
<tr>
<td>12</td>
<td>6.31315</td>
<td>0.2483</td>
<td>6.560E-04</td>
</tr>
<tr>
<td>13</td>
<td>6.33061</td>
<td>0.2484</td>
<td>5.120E-04</td>
</tr>
<tr>
<td>14</td>
<td>6.34440</td>
<td>0.2484</td>
<td>4.075E-04</td>
</tr>
<tr>
<td>15</td>
<td>6.35548</td>
<td>0.2484</td>
<td>3.296E-04</td>
</tr>
</tbody>
</table>

Table 2. The $1s^22p^2\,^3P \, ns\, ^1P$ and $1s^22p^2\,^3P \, nd\, ^1P$ of N IV: energies $E_r$(Ry) (relative to the $1s^22s\,^1S$ of N IV), quantum defect $\mu$, widths $\Gamma$(Ry).

Figure 1 shows the PI cross-section from first ionization threshold $1s^22s\,^1S$ to just above the second threshold $1s^22p\,^3P$, which process corresponding to a 2s electron excited from the ground state $1s^22s\,^1S$ to $2p$ and the others 2s electron excited to $ns$ or $nd$, and form the $1s^22pns\,^1P$ and...
For Review Only

For Review Only

1s22pnd 1P series respectively. The PI cross section of 1s22pnd 1P series is larger than that of 1s22pns 1P series. Energy levels, quantum defect and width calculated by QB method are listed in Table 2. The first resonance of the both series above the first threshold (1s22s 2S) are 1s22p(2P)5s 1P and 1s22p(2P)5d 1P. The first few resonances that correspond to a resonance peak are marked in Figures 1. It is shown that these resonance energy positions are also in good agreement with the results of QB method and experiment results of NIST in Table 2.

For the 1s22p 2P nd 1P series, the effective quantum number is greater than the main quantum number in table 2, this is because the double excited electron 2p and nd electron have a greater interaction, resulting in d-electron orbit is not through in the core and slightly greater than the normal orbit. A similar situation appears in Table 5 (1s23d 2D nf 1P), Table 7 (1s22p(1P)3P nd 1P) and Table 9(1s2p2 2D nf 1P). The quantum defect is less than the whole series such as 1s23s 2S 6p 1P in Table 3, which indicates that the state is disturbed by the energy states of other series. Similar situations can occur in each series.

Table 3. The 1s23s 2S np 1P of N IV: energies E_r (Ry) (relative to the 1s22s 1S of N IV), quantum defect µ, widths Γ (Ry)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>7.66730</td>
<td>0.2930</td>
<td>7.67745</td>
<td>7.66348</td>
<td>2.238E-02</td>
</tr>
<tr>
<td>4</td>
<td>8.63407</td>
<td>0.3736</td>
<td>8.68436</td>
<td></td>
<td>1.129E-03</td>
</tr>
<tr>
<td>5</td>
<td>9.14620</td>
<td>0.2345</td>
<td></td>
<td>1.543E-03</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>9.37834</td>
<td>0.1809</td>
<td></td>
<td>9.348E-04</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>9.49534</td>
<td>0.2903</td>
<td></td>
<td>3.023E-04</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>9.57797</td>
<td>0.3411</td>
<td></td>
<td>1.595E-03</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>9.63891</td>
<td>0.3088</td>
<td></td>
<td>1.002E-03</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>9.67849</td>
<td>0.3618</td>
<td></td>
<td>1.501E-05</td>
<td></td>
</tr>
</tbody>
</table>

Figure 2 displays the PI cross-section from second ionization threshold 1s22p 2P just above the third threshold 1s23s 2S. This resonance series arise mainly from 1s23s(2S)np 1P. In addition, there are low excited resonance states of 1s23pns, nd 1P and 1s23dn, nf 1P series occur in this energy range. The first few resonances which correspond to a resonance peak are indicated in Figure 2, and it is seen that these resonance energy positions are in good accordance with the results of QB method. The comparisons of the energy levels and quantum defect of resonance state for 1s23s 2S np 1P calculated by QB method and that of 1s23p 1P calculated by using the first-order perturbation theory in Ref.[12] together with some experiments results [11] have been listed in Table 3. As shown in Table 3 ours results are in well accord with the experimental and theoretical values.

![Figure 1](https://mc06.manuscriptcentral.com/cjp-pubs)

![Figure 2](https://mc06.manuscriptcentral.com/cjp-pubs)
Table 4. The $1s^23p^2 P$ $ns \, ^1 P$ and $1s^23p^2 P \, nd \, ^1 P$ of N IV: energies $E_r$(Ry) (relative to the $1s^22s^2 P$ of N IV), quantum defect $\mu$, widths $\Gamma$ (Ry)

<table>
<thead>
<tr>
<th>$n$</th>
<th>$E_r$</th>
<th>$\mu$</th>
<th>$E_r$ [11]</th>
<th>$\Gamma$</th>
<th>$E_r$</th>
<th>$\mu$</th>
<th>$E_r$ [11]</th>
<th>$\Gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>8.19383</td>
<td>0.0628</td>
<td>8.20028</td>
<td>8.17693</td>
<td>1.102E-02</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>8.81473</td>
<td>0.3955</td>
<td>8.87645</td>
<td>9.35331</td>
<td>2.022</td>
<td>3.425E-03</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>9.54689</td>
<td>0.3517</td>
<td>9.59756</td>
<td>0.0427</td>
<td>4.270E-04</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>9.69525</td>
<td>0.2690</td>
<td>9.72175</td>
<td>0.0113</td>
<td>2.864E-04</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>9.77861</td>
<td>0.2990</td>
<td>9.80249</td>
<td>0.0663</td>
<td>5.274E-05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>9.87753</td>
<td>0.3228</td>
<td>9.88661</td>
<td>0.0549</td>
<td>2.575E-03</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>9.90851</td>
<td>0.3049</td>
<td>9.91492</td>
<td>0.1696</td>
<td>3.340E-03</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>9.94316</td>
<td>0.1639</td>
<td>9.95217</td>
<td>0.1155</td>
<td>1.915E-03</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>9.97148</td>
<td>0.1954</td>
<td>9.97963</td>
<td>0.1409</td>
<td>4.229E-05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>9.99472</td>
<td>0.1436</td>
<td>10.0001</td>
<td>0.1470</td>
<td>2.053E-05</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 5. The $1s^23d^2 D \, np \, ^1 P$ and $1s^23d^2 D \, nf \, ^1 P$ of N IV: energies $E_r$(Ry) (relative to the $1s^22s^2 P$ of N IV), quantum defect $\mu$, widths $\Gamma$ (Ry)

<table>
<thead>
<tr>
<th>$n$</th>
<th>$E_r$</th>
<th>$\mu$</th>
<th>$E_r$ [11]</th>
<th>$\Gamma$</th>
<th>$E_r$</th>
<th>$\mu$</th>
<th>$E_r$ [11]</th>
<th>$\Gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>9.07021</td>
<td>0.0745</td>
<td>9.18514</td>
<td>9.29698</td>
<td>0.4402</td>
<td>3.146E-03</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>9.45441</td>
<td>0.0543</td>
<td>9.50984</td>
<td>9.67969</td>
<td>0.1081</td>
<td>4.002E-04</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>9.64622</td>
<td>0.1171</td>
<td>9.70874</td>
<td>9.95850</td>
<td>0.0811</td>
<td>7.939E-04</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>9.76130</td>
<td>0.2119</td>
<td>9.82587</td>
<td>9.96580</td>
<td>0.0811</td>
<td>7.939E-04</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>9.85528</td>
<td>0.0516</td>
<td>9.88674</td>
<td>9.96580</td>
<td>0.1346</td>
<td>2.520E-04</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>9.90172</td>
<td>0.2044</td>
<td>9.91856</td>
<td>9.96580</td>
<td>0.1772</td>
<td>2.746E-04</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>9.94316</td>
<td>0.1639</td>
<td>9.95217</td>
<td>9.96580</td>
<td>0.1155</td>
<td>1.915E-03</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>9.97148</td>
<td>0.1954</td>
<td>9.97963</td>
<td>9.96580</td>
<td>0.1409</td>
<td>4.229E-05</td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>9.99472</td>
<td>0.1436</td>
<td>10.0001</td>
<td>10.0001</td>
<td>0.1470</td>
<td>2.053E-05</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The PI cross sections from third ionization threshold $1s^23s^2 S$ just above the fifth ionization threshold $1s^23d^2 D$ are shown in Figure 3. These processes correspond to a 2s electron excited from the ground state $1s^22s^2 S$ to $3p$, and the other 2s electron excited to $ns$ or $nd$, forming the $1s^23pns \, ^1 P$ and $1s^23pnd \, ^1 P$ series, respectively. Alternatively, these processes may correspond to a 2s electron excited from the ground state $1s^22s^2 S$ to $3d$ and the other 2s electron excited to $np$ or $nf$, forming the $1s^23dnp \, ^1 P$ and $1s^23dnf \, ^1 P$ series, respectively. The first resonance of $1s^23pns$, $nd \, ^1 P$ series above the third threshold ($1s^23s^2 S$) are $1s^23p10s \, ^1 P$ and $1s^23p10d \, ^1 P$, and the first resonance of $1s^23dnp$, $nf \, ^1 P$ series above the fourthly threshold ($1s^23p \, ^2 P$) are $1s^23d17p \, ^1 P$ and
The 1s23d17P are located at near the ionization limit 1s23s2S, so we do not get the position of the both states. We mark the first few resonances which correspond to a resonance peak in Figure 3. The energy levels and quantum defect of resonance state for 1s23pns,nd1P, 1s2dnp,nf1P and some experimental and theoretical results[11] are listed in Tables 4 and 5. It is shown that our results well agree with the experimental or theoretical values.

Table 6. The 1s2s2S np1P of N IV: energies E (Ry) (relative to the 1s2s2 1S of N IV), quantum defect µ, widths Γ (Ry)

<table>
<thead>
<tr>
<th>n</th>
<th>Er</th>
<th>µ</th>
<th>Er Ref.</th>
<th>Γ</th>
<th>Γ Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>30.4609</td>
<td>0.2863</td>
<td>30.3010⁹</td>
<td>5.804E-03</td>
<td>4.799E-3⁹</td>
</tr>
<tr>
<td>3</td>
<td>33.8370</td>
<td>0.2212</td>
<td>33.7540⁹</td>
<td>7.215E-03</td>
<td>5.071E-3⁹</td>
</tr>
<tr>
<td>4</td>
<td>34.7704</td>
<td>0.2515</td>
<td></td>
<td>3.043E-03</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>35.2098</td>
<td>0.2165</td>
<td></td>
<td>3.627E-04</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>35.4340</td>
<td>0.1968</td>
<td></td>
<td>8.248E-05</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>35.5650</td>
<td>0.1804</td>
<td></td>
<td>9.546E-05</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>35.6481</td>
<td>0.1702</td>
<td></td>
<td>1.039E-04</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>35.7029</td>
<td>0.1905</td>
<td></td>
<td>4.292E-06</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>35.7426</td>
<td>0.1951</td>
<td></td>
<td>2.461E-06</td>
<td></td>
</tr>
</tbody>
</table>

a—Ref. [4], b—Ref. [19], c—Ref. [13]

Figure 4 displays the PI cross-section for photon energy from 28 Ry to the ionization threshold 1s2s2S which process corresponds to a 1s electron excited from the ground state 1s2s2 1S to np and forms the 1s2snp1P mainly. In addition, there is low excited resonance state of 1s2s2pns,nd1P series occurs in this energy range. The comparisons between our results of the energy levels and quantum defect calculate by QB method and other results are listed in Table 6. For 1s2s2p1P state, the present resonance position and width are 30.4609 Ry and 5.804E-03 Ry, respectively, which are also in accord with the theoretical results 30.3010 Ry and 4.799E-3 Ry by Zhang et al.[4] using the complex-scaled multireference configuration interaction method. Further, these are also in accord with the calculated results 30.3687 Ry and 4.263E-3 Ry by Hsin et al.[13] basing on the saddle-point complex-rotation method. The experimental results of resonance position and width for 1s2s2p1P are 30.4302 Ry and 6.835E-3 Ry, respectively[19]. For the 1s2s3p1P state, ours resonance position and width are 33.8370 Ry and 7.215E-03 Ry, which are in approximately accord with the 33.7540 Ry and 5.071E-3 Ry calculated by Hsin et al. [13].
Table 7. The $1s^22s^22p^3(3P)^2Pns^1P$ and $1s^22s^22p^3(3P)^2Pnd^1P$ of N IV: energies $E_r$(Ry) (relative to the $1s^22s^21S$ of N IV), quantum defects $\mu$, widths $\Gamma$ (Ry)

<table>
<thead>
<tr>
<th>n</th>
<th>$E_r$</th>
<th>$\mu$</th>
<th>$\Gamma$</th>
<th>$E_r$</th>
<th>$\mu$</th>
<th>$\Gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>34.4980</td>
<td>0.3394</td>
<td>2.487E-03</td>
<td>35.0077</td>
<td>0.0231</td>
<td>2.330E-04</td>
</tr>
<tr>
<td>4</td>
<td>35.5117</td>
<td>0.4176</td>
<td>2.151E-03</td>
<td>35.7675</td>
<td>0.0182</td>
<td>3.980E-05</td>
</tr>
<tr>
<td>5</td>
<td>36.0282</td>
<td>0.3190</td>
<td>2.694E-03</td>
<td>36.1241</td>
<td>0.0223</td>
<td>4.763E-05</td>
</tr>
<tr>
<td>6</td>
<td>36.2585</td>
<td>0.3427</td>
<td>1.166E-03</td>
<td>36.3164</td>
<td>0.0163</td>
<td>9.062E-05</td>
</tr>
<tr>
<td>7</td>
<td>36.4191</td>
<td>0.1329</td>
<td>3.525E-04</td>
<td>36.4325</td>
<td>0.0064</td>
<td>2.807E-04</td>
</tr>
<tr>
<td>8</td>
<td>36.4896</td>
<td>0.2850</td>
<td>2.532E-04</td>
<td>36.5091</td>
<td>0.0113</td>
<td>3.827E-05</td>
</tr>
<tr>
<td>9</td>
<td>36.5468</td>
<td>0.3054</td>
<td>2.893E-04</td>
<td>36.5612</td>
<td>0.0078</td>
<td>4.053E-05</td>
</tr>
<tr>
<td>10</td>
<td>36.5879</td>
<td>0.3133</td>
<td>2.362E-04</td>
<td>36.5986</td>
<td>0.0056</td>
<td>3.119E-05</td>
</tr>
</tbody>
</table>

Table 8. The $1s^22s^22p^3(1P)^2Pns^1P$ and $1s^22s^22p^3(1P)^2Pnd^1P$ of N IV: energies $E_r$(Ry) (relative to the $1s^22s^21S$ of N IV), quantum defects $\mu$, widths $\Gamma$ (Ry)

<table>
<thead>
<tr>
<th>n</th>
<th>$E_r$</th>
<th>$\mu$</th>
<th>$\Gamma$</th>
<th>$E_r$</th>
<th>$\mu$</th>
<th>$\Gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>34.8267</td>
<td>0.3520</td>
<td>2.159E-03</td>
<td>35.2808</td>
<td>0.0413</td>
<td>3.573E-03</td>
</tr>
<tr>
<td>4</td>
<td>35.9504</td>
<td>0.2832</td>
<td>1.466E-03</td>
<td>36.0885</td>
<td>0.0396</td>
<td>4.165E-03</td>
</tr>
<tr>
<td>5</td>
<td>36.3798</td>
<td>0.3145</td>
<td>8.252E-04</td>
<td>36.4598</td>
<td>0.0340</td>
<td>2.156E-03</td>
</tr>
<tr>
<td>6</td>
<td>36.6069</td>
<td>0.3527</td>
<td>1.039E-03</td>
<td>36.6577</td>
<td>0.0431</td>
<td>1.319E-03</td>
</tr>
<tr>
<td>7</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>36.7895</td>
<td>0.0315</td>
<td>8.671E-03</td>
</tr>
<tr>
<td>8</td>
<td>36.8321</td>
<td>0.3925</td>
<td>4.906E-04</td>
<td>36.8570</td>
<td>0.0259</td>
<td>8.952E-04</td>
</tr>
<tr>
<td>9</td>
<td>36.8896</td>
<td>0.4516</td>
<td>7.554E-04</td>
<td>36.9094</td>
<td>0.0375</td>
<td>6.081E-04</td>
</tr>
<tr>
<td>10</td>
<td>36.9384</td>
<td>0.3043</td>
<td>3.009E-04</td>
<td>36.9473</td>
<td>0.0399</td>
<td>3.836E-04</td>
</tr>
</tbody>
</table>

Figures 5 and 6 show the PI cross-section from $1s^22s^22S$ to the ionization threshold $1s^22s2p^3(3P)^2P$ and from $1s^22s2p^3(1P)^2P$ to $1s^22s2p^3(1P)^2P$ ionization threshold respectively, of which process corresponds to a $1s$ electron excited from the ground state $1s^22s^21S$ to $2p$ and a $2s$ electron excited to $ns$ or $nd$, forming the $1s^22s2p^32Pns^1P$ and $1s^22s2p^32Pnd^1P$ series, respectively. In addition, there are low excited resonance states of $1s^22s2p^3(1P)^2Pns^1P$ and $1s^22s2p^3(1P)^2Pnd^1P$ series occur in the energy range of Figure 5 and some excited resonance states of $1s^2p^32Dnp, nf^1P$ series in the energy range of Figure 6 respectively. The energy levels and quantum defect of resonance state for $1s^22s2p^32Pns^1P$ and $1s^22s2p^32Pnd^1P$ series calculated by QB method are listed in Table 7 and Table 8.
Table 9. The $1s2p^2 \, ^2D \, np \, ^1P$ and $1s2p^2 \, ^2D \, nf \, ^1P$ of N IV: energies $E_r$(Ry) (relative to the $1s^22s^2 \, ^1S$ of N IV), quantum defect $\mu$, widths $\Gamma$ (Ry)

<table>
<thead>
<tr>
<th>$n$</th>
<th>$E_r$</th>
<th>$\mu$</th>
<th>$E_r$ [13]</th>
<th>$\Gamma$</th>
<th>$E_r$</th>
<th>$\mu$</th>
<th>$\Gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>32.4777</td>
<td>0.1896</td>
<td>32.2766</td>
<td>3.810E-03</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>35.3698</td>
<td>0.1642</td>
<td>36.3741</td>
<td>0.0296</td>
<td>9.223E-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>36.2770</td>
<td>0.1554</td>
<td>36.7294</td>
<td>0.0392</td>
<td>1.675E-05</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>36.6859</td>
<td>0.1262</td>
<td>36.9216</td>
<td>0.0449</td>
<td>7.019E-05</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>36.9034</td>
<td>0.0770</td>
<td>37.0364</td>
<td>0.037</td>
<td>7.956E-05</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>37.0253</td>
<td>0.0804</td>
<td>8.007E-04</td>
<td>37.0364</td>
<td>0.037</td>
<td>7.383E-05</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>37.1117</td>
<td>0.0393</td>
<td>9.851E-05</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>37.1566</td>
<td>0.1198</td>
<td>2.454E-03</td>
<td>37.1634</td>
<td>0.0347</td>
<td>7.383E-05</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>37.1945</td>
<td>0.1507</td>
<td>1.431E-03</td>
<td>37.2005</td>
<td>0.0320</td>
<td>6.707E-05</td>
<td></td>
</tr>
</tbody>
</table>

Table 10. The $1s2p^2 \, ^2P \, np \, ^1P$ and $1s2p^2 \, ^2S \, np \, ^1P$ of N IV; energies $E_r$(Ry) (relative to the $1s^22s^2 \, ^1S$ of N IV), quantum defect $\mu$, widths $\Gamma$ (Ry)

<table>
<thead>
<tr>
<th>$n$</th>
<th>$E_r$</th>
<th>$\mu$</th>
<th>$\Gamma$</th>
<th>$E_r$</th>
<th>$\mu$</th>
<th>$\Gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>35.5117</td>
<td>0.1357</td>
<td>2.151E-03</td>
<td>35.9504</td>
<td>0.1574</td>
<td>1.466E-03</td>
</tr>
<tr>
<td>4</td>
<td>36.3835</td>
<td>0.1482</td>
<td>1.226E-03</td>
<td>36.8507</td>
<td>0.1506</td>
<td>1.722E-04</td>
</tr>
<tr>
<td>5</td>
<td>36.7855</td>
<td>0.1165</td>
<td>1.523E-02</td>
<td>37.2436</td>
<td>0.1736</td>
<td>1.606E-03</td>
</tr>
<tr>
<td>6</td>
<td>36.9971</td>
<td>0.1130</td>
<td>1.788E-03</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>7</td>
<td>37.1239</td>
<td>0.1201</td>
<td>3.263E-03</td>
<td>37.5874</td>
<td>0.1709</td>
<td>2.083E-03</td>
</tr>
<tr>
<td>8</td>
<td>37.2043</td>
<td>0.1193</td>
<td>2.253E-03</td>
<td>37.6695</td>
<td>0.1707</td>
<td>1.363E-03</td>
</tr>
<tr>
<td>9</td>
<td>37.2591</td>
<td>0.1183</td>
<td>1.377E-03</td>
<td>37.7252</td>
<td>0.1705</td>
<td>9.069E-04</td>
</tr>
<tr>
<td>10</td>
<td>37.2983</td>
<td>0.1115</td>
<td>9.183E-04</td>
<td>37.7649</td>
<td>0.1704</td>
<td>6.538E-04</td>
</tr>
</tbody>
</table>

The PI cross sections from ionization threshold $1s2s2p(^1P)^2P$ to the ionization threshold $1s2p^2 \, ^2P$ are plotted in Figure 7, which corresponds to the $1s2p^2 \, ^2D \, np$, $nf \, ^1P$ and $1s2p^2 \, ^2P \, np \, ^1P$ series, respectively. The comparisons between our results of the energy levels and quantum defect calculated by QB method and other calculated results have been tabulated in Table 9. Moreover, Hsin et al.[13] have studied the $1s2p^3 \, ^1P$ resonances from $1s^22s^2 \, ^1S$ using the saddle-point
complex-rotation method, and the results are $E_r=32.2766$ Ry and $\Gamma=3.16\text{E-3}$, which are consistent with the present results $32.4777$ Ry and $3.81\text{E-3}$.

Figure 8 shows the PI cross section from $1s2p^2\,^2P$ to the ionization threshold $1s2p^2\,^2S$, which corresponds to the $1s2p^2\,^2S\,np\,^1P$ and the energy levels and quantum defect calculated by QB method listed in Table 10. Since the position of the $1s2p^2\,^2D\,8p\,^1P$ is close to the ionization threshold $1s2s2p\,(^1P)^2P$, and the position of $1s2p^2\,^2S\,6p\,^1P$ is close to the ionization threshold $1s2p^2\,^2D$, we have not obtained the energy of $1s2p^2\,^2D\,8p\,^1P$ and $1s2p^2\,^2S\,6p\,^1P$.

Table 11. The $1s2s(^3S)3s\,^2S\,np\,^1P$ and $1s2s(^1S)3s\,^2S\,np\,^1P$ of N IV: energies $E_r$(Ry) (relative to the $1s^22s\,^1S$ of N IV), quantum defect $\mu$, widths $\Gamma$(Ry)

<table>
<thead>
<tr>
<th>n</th>
<th>$E_r$</th>
<th>$\mu$</th>
<th>$\Gamma$</th>
<th>$E_r$</th>
<th>$\mu$</th>
<th>$\Gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>38.3445</td>
<td>0.3940</td>
<td>1.189E-02</td>
<td>39.0363</td>
<td>0.2421</td>
<td>9.422E-03</td>
</tr>
<tr>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>39.9706</td>
<td>0.3182</td>
<td>1.373E-03</td>
<td>40.4097</td>
<td>0.3191</td>
<td>6.545E-04</td>
</tr>
<tr>
<td>6</td>
<td>40.2085</td>
<td>0.2977</td>
<td>5.650E-04</td>
<td>40.6472</td>
<td>0.3017</td>
<td>4.110E-04</td>
</tr>
<tr>
<td>7</td>
<td>40.3451</td>
<td>0.2909</td>
<td>3.565E-04</td>
<td>40.7839</td>
<td>0.2964</td>
<td>3.019E-04</td>
</tr>
<tr>
<td>8</td>
<td>40.4316</td>
<td>0.2871</td>
<td>2.613E-04</td>
<td>40.8705</td>
<td>0.2941</td>
<td>2.032E-04</td>
</tr>
<tr>
<td>9</td>
<td>40.4899</td>
<td>0.2849</td>
<td>1.735E-04</td>
<td>40.9289</td>
<td>0.2930</td>
<td>1.426E-04</td>
</tr>
<tr>
<td>10</td>
<td>40.5311</td>
<td>0.2831</td>
<td>1.248E-04</td>
<td>40.9702</td>
<td>0.2914</td>
<td>1.035E-04</td>
</tr>
</tbody>
</table>

The PI cross sections for photon energy from 38.1 Ry to the ionization threshold $1s2s(^3S)3s\,^2S$ are shown in Figure 9 which corresponds to the $1s2s(^3S)3s\,^2S\,np\,^1P$ and $1s2s(^1S)3s\,^2S\,np\,^1P$ series, respectively, and the corresponding energy levels and quantum defect are listed in Table 11. When $n=3-6$, the PI cross sections of $1s2s(^3S)3s\,^2S\,np\,^1P$ and $1s2s(^1S)3s\,^2S\,np\,^1P$ are small and almost coincide with the background, so we have not obtained the energy of $1s2s(^3S)3s\,^2S\,4p\,^1P$ and $1s2s(^1S)3s\,^2S\,4p\,^1P$ using QB method.

4. Conclusions

Ab initio calculations of PI cross sections have been carried out using the Breit-Pauli $R$-matrix method in the $LS$-coupling approximation combined with the relativistic distorted-wave method and QB method. In present work, we calculated the PI cross sections of N IV for ejection of two $2s$ or ejection of a $1s$ and a $2s$ electrons from the ground state $1s^22s\,^1S$ to form the state of $^1P$ of nineteen series. Our results are in excellent agreement with the existing experimental and the latest theoretical results. We believe that our results are the most extensive and accurate to date and
should be useful in the study of astrophysical plasmas.

Reference


[4] Zhang SB and Danny LY. Complex-scaled multireference configuration-interaction method to study Be and Be-like cations(B, C, N, O, Mg) Auger resonances 1s2s2p 3^3P^o. PHYSICAL REVIEW A 2012:85; 032515.


[8] Pedro Amaro, Filippo Fratini etc., Relativistic evaluation of the two-photon decay of the metastable 1s^22s p 3^3P^o state in berylliumlike ions with an effective-potential model. PHYSICAL REVIEW A 2016:93; 032502.


[13] Hsin Lin, Chen-Shiung Hsue, and Kwong T. Chung, Auger width and branching ratios for berylliumlike 1s2s^np 1^P^o and 1s2p^3 1^P^o resonances and photoionization of beryllium from 1s^22s^2 1^S, PHYSICAL REVIEW A, 2002:65; 032706.


[17] Burke PG, Noble CJ and Burke VM. R-Matrix Theory of Atomic, Molecular and Optical
