STUDIES OF PHOTOIONIZATION PROCESSES OF NITROGEN-LIKE O’ION USING THE SCREENING CONSTANT BY UNIT NUCLEAR CHARGEMETHOD

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Abstract

In this present work, we have calculated the energies positions of the 2s²²p²(1D)nd²P, 2s²²p²(1D)nd²S, 2s²²p²(1D)nd²D, 2s²²p²(1S)nd²P and 2s²²p²(1P)nd²D Rydberg series in the photoionization spectra from the ³P° metastable state of the O’ ion. Calculations were performed up to n = 40 applying the Screening Constant by Unit Nuclear Charge (SCUNC) via its semi empirical formalism. The quantum defect and the effective charge are also calculated. The results agree within 98% to Aguilar’s experimental data, and with Sow’s theoretical results to within 99%. These data can be a useful guideline for future experimental and theoretical studies.

Introduction:

Due to its existence in the earth’s atmosphere as well as in many astrophysical objects, oxygen is one of the most important elements in nature. For the modeling of astrophysical and laboratory plasmas, it is imperative to provide precise photoionization data. Thus, for decades, absolute photoionization cross-section calculations of ions have been carried out using different approximations and techniques. For the oxygen atom, theoretical and experimental studies on the K–shell photoionization [1–5] have been carried out. However, for oxygen ions, most of the experimental and theoretical studies of photoionization lie in the photons energy range of vacuum ultraviolet [6].

To reestimate the stellar envelope opacities in terms of atomic data computed by ab initio methods [7–8], the atomic database called the Opacity Project (OP) was formed at the Strasbourg Astronomical Data Center in France in 1981 [9]. Combining the projects OP, OPAL [10–11] and Iron [12], several atomic databases widely used for astrophysical calculations were born. In recent years, the study of the photoionization of atomic ions has made great progress. For a summary of this progress, see the recent comprehensive review by West 2001 [13]. Photoabsorption processes from low-lying metastable states of open-shell nitrogen–like ions are particularly important in astrophysical plasmas as well as in the upper atmosphere [14].

Covington et al. [15] have performed high-resolution absolute experimental measurements for the photoionization of O+ ions from ³P° and ³D° metastable states and from the ³S° ground state in the photon energy range 30–35.5 eV. To interpret the experiment, theoretical calculations have been carried out and the result show that the cross-sections are sensitive to the choice of basis states. Kjeldsen et al. [16] have also measured the absolute photoionization cross-sections in region of 30–150 eV by fusing a synchrotron radiation beam from an undulator with a 2 keV ions beam. Thus, Aguilar et al. [9] performed the absolute photoionization of O° from 29.7 to 46.2 eV above the first ionization...
threshold, using a merged–beam line at the Advanced Light Source (ALS). More recently, Sow et al. [17] calculated the energies positions of some Rydberg series from the \(^5\)P\(^\pm\) metastable state of \(O^+\) ions using the Modified Orbital Atomic Theory (MAOT). These data are very useful for interpreting and simulating absorption or emission spectra for both astrophysical and laboratory plasmas. They are also helpful for analyzing the Auger spectra of \(O^+\) ions.

In order to provide useful data and to prove the validity of the Screening Constant by Unit Nuclear Charge (SCUNC) in the study of the photoionization of atomic ions, we have calculated in this paper, the resonance energies of the \(2s^22p^2(\text{D})n\text{d}^\text{f} \text{'D}, 2s^22p^2(\text{D})n\text{s}^\text{2S}, 2s^22p^2(\text{D})n\text{d}^\text{2D}, 2s^22p^2(\text{D})\text{n}^\text{2P} \text{D} \text{Rydberg series of the nitrogen–like ion O}^+ up to n = 40 using the SCUNC–method via its semi–empirical formalism. Energies resonances are compared to the experimental data [9] and theoretical data [17]. To analyze the results, we report the quantum defect and the effective charge.

Theory

Brief description of the SCUNC formalism

In the framework of the SCUNC formalism, the resonance energy of a given Rydberg series originating from \(2S + 1\)\(^L\)\(^S\) state, is given by [18–19]:

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

In this equation, \(\nu\) and \(\mu\) (\(\mu > \nu\)) denote the principal quantum numbers of the \((2S + 1)\text{L}\text{S}\) Rydberg series used in the empirical determination of the \(f_i\)-screening constants, \(s\) represents the spin of the \(n\text{l}\)-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:

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

Where \(f_k(2S + 1)^L_S, n, s, \mu, \nu\) are screening constants to be evaluated empirically. In Eq.(2), \(q\) stands for the number of terms in the expansion of the \(\beta\)-parameters. Generally, precise resonance energies are obtained for \(q < 5\). The resonance energy are the in the form:

\[
E_{n} = E_{\infty} - \frac{Z^2}{n^2} \left\{1 - \frac{f_i(2S + 1)^L_S}{Z(n - 1)} - \frac{f_i(2S + 1)^L_S}{Z} \pm \sum_{k=1}^{q} \sum_{k'=1}^{q'} f_k' F(n, \nu, \mu, s) \times \left(\frac{1}{Z}\right)^k\right\}^2
\] (3)

The quantity \(\sum_{k=1}^{q} \sum_{k'=1}^{q'} f_k' F(n, \nu, \mu, s) \times \left(\frac{1}{Z}\right)^k\) is a corrective term introduce to stabilize the resonance energies with increasing the principal quantum number \(n\).

Besides, resonance energies are generally analyzed from the standard quantum defect expansion formula:

\[
E_{n} = E_{\infty} - \frac{RZ^2_{\text{con}}}{(n - \delta)^2}
\] (4)

In this equation, \(R\) is the Rydberg constant, \(E_{\infty}\) denotes the converging energy limit, \(Z_{\text{con}}\) represents the electric charge of the 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:

\[
E_{n} = E_{\infty} - \frac{Z^2}{n^2} R
\] (5)

In this equation, \(Z^* = Z_{\infty} \left\{1 - F \left[f_i(2S + 1)^L_S, n, \nu, \mu, s, Z\right]\right\}.

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

\[
Z^* = \frac{Z_{\text{con}}}{\left(1 - \frac{\delta}{n}\right)}
\] (6)
According to this equation, each Rydberg series must satisfy the following conditions:

\[
\begin{align*}
Z^* & \geq Z_{C} \quad \text{if} \quad \delta \geq 0 \\
Z^* & \leq Z_{C} \quad \text{if} \quad \delta \leq 0 \quad (7)
\end{align*}
\]

\[
\lim_{n \to \infty} Z^* = Z_C
\]

Besides, comparing Eq.(3) and Eq.(5), the effective charge is in the form

\[
Z^* = Z \left(1 - \frac{f_1(2\nu + L^2)}{Z(n-1)} - \frac{f_2(2\nu + L^2)}{Z} \right) + \sum_{\nu=1}^{\delta} \sum_{\nu'=1}^{\delta} \frac{f_1}(n, \nu, \mu, \nu', \mu, \nu) \left(\frac{1}{Z}\right)^{\delta}
\]

Besides, the \( f_2 \)-parameter in Eq. (3) can be theoretically determined from the equation

\[
\lim_{n \to \infty} Z^* = Z \left(1 - \frac{f_2(2\nu + L^2)}{Z}\right) = Z_{\text{core}} \quad (9)
\]

We get then \( f_2 = Z - Z_{\text{core}} \), where \( Z_{\text{core}} \) is directly obtain from the photoionization process of a given atomic \( X''' \) system: \( X''' + h\nu \rightarrow X'''' + e^- \)  

We find then \( Z_{\text{core}} = m+1 \). As an illustration for \( O^+ \) we have \( h\nu + O^+ \rightarrow O^{2+} + e^- \). So, for the \( O^+ \) ion, \( f_2 = 6.00 \).

The remaining \( f_1 \)-parameter is then to be evaluated empirically using experimental data for a given \( ^{(2\nu + L^2)}\) level with \( n = 0 \) in Eq. (3) as shown previously [20].

### Energy Resonances of the \( 2s^22p^2(1D)ns^2D \), \( 2s^22p^2(1D)ns^2S \), \( 2s^22p^2(1S)nd^2D \) and \( 2s2p^3(1P)np^3D \)

In the framework of the SCUNC formalism, the resonances energies for the different Rydberg series studied for the Nitrogen–like \( O^+ \) ion are given by (in Rydberg units):

- For the Rydberg series \( 2s^22p^2(1D)nd^2P \) from the \( ^2P^* \) Metastable state

\[
E_n = E_{n^0} - \frac{Z^2}{n^2} \left(1 - \frac{f_1(2P)}{Z(n-1)} - \frac{f_2(2P)}{Z} \right) - \frac{f_1(2P)(n-\mu)}{Z^2(n+\mu-s-2)(n+2s)} - \frac{f_1(2P)(n-\mu)}{Z^3(n+\mu-s-1)^2} \quad (10)
\]

- For the Rydberg series \( 2s^22p^2(1D)nd^2S \) from the \( ^2P^* \) Metastable state

\[
E_n = E_{n^0} - \frac{Z^2}{n^2} \left(1 - \frac{f_1(2S)}{Z(n-1)} - \frac{f_2(2S)}{Z} \right) - \frac{f_1(2S)(n-\mu)}{Z^2(n+\mu-s-2)(n+2s)} - \frac{f_1(2S)(n-\mu)}{Z^3(n+\mu-s-1)^2} \quad (11)
\]

- For the Rydberg series \( 2s^22p^2(1D)ns^2D \) from the \( ^2P^* \) Metastable state

\[
E_n = E_{n^0} - \frac{Z^2}{n^2} \left(1 - \frac{f_1(2D)}{Z(n-1)} - \frac{f_2(2D)}{Z} \right) - \frac{f_1(2D)(n-\mu)}{Z^2(n+\mu+s)^2} - \frac{f_1(2D)(n-\mu)}{Z^3(n+\mu+s+2)^2} \quad (12)
\]

The \( f_{(2L)} \) screening constants are evaluated using the experimental data of ALS energies of Aguilar and al. [9]. For the \( 2s^22p^2(1D)5d^2P(\mu = 5), 2s^22p^2(1D)5d^2S(\mu = 5) \) and \( 2s^22p^2(1D)6s^2D(\mu = 6) \) levels respectively at (in eV) 30.393, 30.213 and 30.578. As far as energy limit is concerned, he is equal to 32.617 eV (NIST) [21]. We find from Eq.(10) \( f_{(2P)} = -0.086 \), from Eq.(11) \( f_{(2S)} = -0.050 \) and from Eq.(12) \( f_{(2D)} = -1.614 \).
The present results obtained for the resonance energies $E$, quantum defect $\delta$ and effective charge $Z^*$ of the $2s^22p^2(1D)nd^2P$, $2s^22p^2(1D)ns^2D$ and $2s^22p^2(1D)ns^2D$ series of $O^+$ are quoted in Table 1.

- For the Rydberg series $2s^22p^2(1S)nd^2D$ from the $2P^o$ Metastable state

$$E_n = E_{\infty} - \frac{Z^2}{n^2} \left[ 1 - \frac{f_1(1S)}{Z(n-1)} - \frac{f_2(1S)}{Z(n+\mu-s)} + \cdots \right]$$

**Eqs. (13) and (14)**

The value of $f_1(1S)$ is evaluated from ALS experiments of Aguilar and al. [9] for the $2s^22p^2(1S)4d^2D$ ($\mu = 4$), $E_4 = 31.924$ eV. Using $E_{\infty} = 35.458$ eV from NIST [21], Eq.(13) gives then $f_1(1S) = -0.116$.

- For the Rydberg series $2s2p^3(3P)np^2D$ from the $2P^o$ Metastable state

$$E_n = E_{\infty} - \frac{Z^2}{n^2} \left[ 1 - \frac{f_1(3P)}{Z(n-1)} - \frac{f_2(3P)}{Z(n+\mu-s)} - \frac{f_3(3P)}{Z^3(n+\mu+s+1)} \right]$$

Besides, the value of $f_1(3P)$ is evaluated from ALS experiments of Aguilar and al. [9] for the $2s^22p^2(3P)3p^2D$ ($\mu = 3$), $E_3 = 39.478$ eV. Using $E_{\infty} = 47.527$ eV from NIST [21], Eq.(14) gives then $f_1(3P) = -0.615$.

The present results obtained for the resonance energies $E$, quantum defect $\delta$ and effective charge $Z^*$ of the $2s^22p^2(1S)nd^2D$ and $2s^22p^2(1P)np^2D$ series of $O^+$ are quoted in Table 2.

**Results And Discussions:-**

In this present article, the calculations of the resonance energies reported for photoionization of the $2P^o$ metastable states of the $O^+$ ion have been extended to $n = 40$ and the results obtained are presented in Tables 1 and 2. Tables 3 and 4 compare the current results calculated with the Screening Constant by Unit Nuclear Charge (SCUNC) method, with the theoretical predictions (MOAT) of Sow et al. [17], and the Advanced Light Source experimental data of Aguilar et al. [9]. This comparison is also made by calculating the relative differences ($Diff\%$).

In the framework of the SCUNC formalism, Eq.(4) shows that the precision of the calculations of $E_n$ depends on the precision on the calculations of $E_{\infty}$ and of $Z^*$. Gao et al. [22] reported that, relativistic effects, quantum electrodynamic contributions (QED) and nuclear size effects increase with higher powers of the charge state of highly charged ions. So, let's move on to discussing the accuracy of current calculations with respect to $Z^*$. For this, the value of $Z_{\text{core}}$ deduced from the photoionization process of the $O^+$ ion ($O^+ + h\nu \rightarrow O^+++ e^+$) gives $Z_{\text{core}} = 2$. For this, we have studied the behavior of the effective nuclear charge $Z^*$ and of the quantum defect $\delta$. In Tables 1 and 2, we see that $Z^* \geq Z_{\text{core}}$ so quantum defects are positive according to the SCUNC analysis conditions Eq.(7). In addition, along the series, the current quantum defect is almost constant. All this shows, on the one hand, that the results of the SCUNC cited in Tables 1 and 2 are sufficiently precise and can constitute good guidelines for investigators in the field.

In Table 3, we compare our results on the resonance energies (in eV) of the $2s^22p^2(1D)nd^2P$ and $2s^22p^2(1D)ns^2D$ Rydberg series from the $2P^o$ metastable state of the $O^+$ ion with the experimental and theoretical data. It can easily be seen that a good agreement is found with the experimental data of Aguilar et al. [9] and the theoretical results of Sow et al. [17]. For the energies of the $2s^22p^2(1D)nd^2P$ states, the relative differences being $< 0.03\%$ compared to the experimental data and $< 0.05\%$ compared to the theoretical data. While for $2s^22p^2(1D)ns^2D$ states, the relative differences are $< 0.01\%$ to both experimental and theoretical data.

Table 4 shows a comparison of the resonance energies of the $2s^22p^2(1S)nd^2P$ and $2s2p^3(1P)np^2D$ from the $2P^o$ metastable state of the $O^+$ ion compared to the experimental data [9] and theoretical [17]. For the energies of the $2s^22p^2(1S)nd^2D$ states, the maximum relative difference from the experimental and theoretical data is 0.04. This indicates the excellent agreement between our present results and the other data. Moreover, for $n \geq 16$, it should be
emphasized that the SCUNC method exactly reproduces the theoretical results [17]. This is explained by the fact that both methods used the semi-empirical formalism. For 2s2p(1P)mpD states, again, the chords are perceived as very good. It should be noted that for this Rydberg series, the results are less precise compared to the other series studied. This is explained by the fact that, the limit energy and the energy of the 2s2p(1P)mpD state that we have used for the determination of the screening constant f(L) are questionable (See Aguilar et al. [9]). And as we have already stated above, in the SCUNC formalism, the precision of the calculations of E_n depends on the precision of the limit energies E_o.

These good agreements are justified by the fact that, in the SCUNC formalism, all the relativistic and electron-electron correlation effects are implicitly taken into account in the adjustment parameters f_k evaluated using experimental data.

Table 1: Resonances energies (E, eV), quantum defect (δ) and effective charge (Z*) of the 2s2p(1D)mpD, 2s2p(1P)mpS and 2s2p(1S)msD Rydberg series from the P^+ Metastable state of O^+.

| States n | 2s2p(1D)mpD | 2s2p(1P)mpS | 2s2p(1S)msD |
|---------|-------------|-------------|-------------|
|         | E   | δ   | Z* | E   | δ   | Z* | E   | δ   | Z* |
| 5       | 30.393 | 0.05 | 2.02 | 30.413 | 0.03 | 2.01 | 30.578 | 0.83 | 2.32 |
| 6       | 31.079 | 0.05 | 2.02 | 31.090 | 0.03 | 2.01 | 31.188 | 0.83 | 2.27 |
| 7       | 31.490 | 0.05 | 2.01 | 31.497 | 0.03 | 2.01 | 31.559 | 0.83 | 2.23 |
| 8       | 31.756 | 0.05 | 2.01 | 31.760 | 0.03 | 2.01 | 31.802 | 0.83 | 2.20 |
| 9       | 31.938 | 0.05 | 2.01 | 31.941 | 0.03 | 2.01 | 31.970 | 0.83 | 2.18 |
| 10      | 32.067 | 0.05 | 2.01 | 32.070 | 0.03 | 2.01 | 32.091 | 0.83 | 2.16 |
| 11      | 32.163 | 0.05 | 2.01 | 32.165 | 0.03 | 2.01 | 32.181 | 0.83 | 2.15 |
| 12      | 32.236 | 0.05 | 2.01 | 32.237 | 0.03 | 2.00 | 32.250 | 0.83 | 2.14 |
| 13      | 32.293 | 0.05 | 2.01 | 32.294 | 0.03 | 2.00 | 32.303 | 0.83 | 2.13 |
| 14      | 32.337 | 0.05 | 2.01 | 32.338 | 0.03 | 2.00 | 32.346 | 0.83 | 2.12 |
| 15      | 32.374 | 0.05 | 2.01 | 32.374 | 0.03 | 2.00 | 32.380 | 0.83 | 2.11 |
| 16      | 32.403 | 0.05 | 2.01 | 32.404 | 0.03 | 2.00 | 32.409 | 0.83 | 2.10 |
| 17      | 32.428 | 0.05 | 2.01 | 32.428 | 0.03 | 2.00 | 32.432 | 0.83 | 2.10 |
| 18      | 32.448 | 0.05 | 2.01 | 32.449 | 0.03 | 2.00 | 32.452 | 0.83 | 2.09 |
| 19      | 32.465 | 0.05 | 2.01 | 32.466 | 0.03 | 2.00 | 32.469 | 0.84 | 2.09 |
| 20      | 32.480 | 0.05 | 2.00 | 32.481 | 0.03 | 2.00 | 32.483 | 0.84 | 2.08 |
| 21      | 32.493 | 0.05 | 2.00 | 32.493 | 0.03 | 2.00 | 32.495 | 0.84 | 2.08 |
| 22      | 32.504 | 0.05 | 2.00 | 32.504 | 0.03 | 2.00 | 32.506 | 0.84 | 2.08 |
| 23      | 32.514 | 0.05 | 2.00 | 32.514 | 0.03 | 2.00 | 32.516 | 0.84 | 2.07 |
| 24      | 32.522 | 0.05 | 2.00 | 32.522 | 0.03 | 2.00 | 32.524 | 0.84 | 2.07 |
| 25      | 32.530 | 0.05 | 2.00 | 32.530 | 0.03 | 2.00 | 32.531 | 0.84 | 2.07 |
| 26      | 32.536 | 0.05 | 2.00 | 32.536 | 0.03 | 2.00 | 32.537 | 0.84 | 2.06 |
| 27      | 32.542 | 0.05 | 2.00 | 32.542 | 0.03 | 2.00 | 32.543 | 0.84 | 2.06 |
| 28      | 32.547 | 0.05 | 2.00 | 32.547 | 0.03 | 2.00 | 32.548 | 0.84 | 2.06 |
| 29      | 32.552 | 0.05 | 2.00 | 32.552 | 0.03 | 2.00 | 32.553 | 0.85 | 2.06 |
| 30      | 32.556 | 0.05 | 2.00 | 32.556 | 0.03 | 2.00 | 32.557 | 0.85 | 2.06 |
| 31      | 32.560 | 0.05 | 2.00 | 32.560 | 0.03 | 2.00 | 32.561 | 0.85 | 2.05 |
| 32      | 32.564 | 0.05 | 2.00 | 32.564 | 0.03 | 2.00 | 32.564 | 0.85 | 2.05 |
| 33      | 32.567 | 0.05 | 2.00 | 32.567 | 0.03 | 2.00 | 32.567 | 0.85 | 2.05 |
| 34      | 32.570 | 0.05 | 2.00 | 32.570 | 0.03 | 2.00 | 32.570 | 0.85 | 2.05 |
| 35      | 32.572 | 0.05 | 2.00 | 32.573 | 0.03 | 2.00 | 32.573 | 0.85 | 2.05 |
| 36      | 32.575 | 0.05 | 2.00 | 32.575 | 0.03 | 2.00 | 32.575 | 0.85 | 2.05 |
| 37      | 32.577 | 0.05 | 2.00 | 32.577 | 0.03 | 2.00 | 32.578 | 0.85 | 2.05 |
| 38      | 32.579 | 0.05 | 2.00 | 32.579 | 0.03 | 2.00 | 32.580 | 0.85 | 2.04 |
| 39      | 32.581 | 0.05 | 2.00 | 32.581 | 0.03 | 2.00 | 32.581 | 0.85 | 2.04 |
| 40      | 32.583 | 0.05 | 2.00 | 32.583 | 0.03 | 2.00 | 32.583 | 0.85 | 2.04 |
| ...     | ...    | ...    | ... | ...    | ...    | ... | ...    | ...    | ... |
| ∞       | 32.617 | 2.00 |    | 32.617 | 2.00 |    | 32.617 | 2.00 |    |
Table 2: Resonances energies \((E, \text{ eV})\), quantum defect \((\delta)\) and effective charge \((Z^*)\) of the \(2s^22p^2(1S)nd^2D\) and \(2s2p^2(1P)np^2D\) Rydberg series from the \(^1P^\ast\) Metastable state of \(\text{O}^+\).

| States \(n\) | \(2s^22p^2(1S)nd^2D\) | \(E\) | \(\delta\) | \(Z^*\) | \(2s2p^2(1P)np^2D\) | \(E\) | \(\delta\) | \(Z^*\) |
|-----------|------------------|------|-----|-------|------------------|------|-----|-------|
| 3         | 31.924           | 0.08 | 2.04|       | 39.478           | 0.40 | 2.31|       |
| 4         | 33.217           | 0.07 | 2.03|       | 43.391           | 0.37 | 2.21|       |
| 5         | 33.910           | 0.07 | 2.02|       | 45.000           | 0.36 | 2.15|       |
| 6         | 34.325           | 0.07 | 2.02|       | 46.298           | 0.35 | 2.10|       |
| 7         | 34.593           | 0.07 | 2.02|       | 46.599           | 0.34 | 2.09|       |
| 8         | 34.776           | 0.07 | 2.02|       | 46.801           | 0.34 | 2.08|       |
| 9         | 34.906           | 0.07 | 2.01|       | 46.944           | 0.34 | 2.07|       |
| 10        | 35.003           | 0.07 | 2.01|       | 47.048           | 0.34 | 2.06|       |
| 11        | 35.076           | 0.07 | 2.01|       | 47.127           | 0.34 | 2.06|       |
| 12        | 35.133           | 0.07 | 2.01|       | 47.188           | 0.34 | 2.05|       |
| 13        | 35.178           | 0.07 | 2.01|       | 47.236           | 0.34 | 2.05|       |
| 14        | 35.214           | 0.07 | 2.01|       | 47.274           | 0.34 | 2.05|       |
| 15        | 35.244           | 0.07 | 2.01|       | 47.305           | 0.34 | 2.04|       |
| 16        | 35.268           | 0.07 | 2.01|       | 47.331           | 0.34 | 2.04|       |
| 17        | 35.289           | 0.07 | 2.01|       | 47.353           | 0.34 | 2.04|       |
| 18        | 35.306           | 0.07 | 2.01|       | 47.371           | 0.34 | 2.04|       |
| 19        | 35.321           | 0.07 | 2.01|       | 47.386           | 0.34 | 2.03|       |
| 20        | 35.334           | 0.07 | 2.01|       | 47.400           | 0.34 | 2.03|       |
| 21        | 35.345           | 0.07 | 2.01|       | 47.411           | 0.34 | 2.03|       |
| 22        | 35.355           | 0.07 | 2.01|       | 47.421           | 0.34 | 2.03|       |
| 23        | 35.363           | 0.07 | 2.01|       | 47.430           | 0.34 | 2.03|       |
| 24        | 35.370           | 0.07 | 2.01|       | 47.438           | 0.34 | 2.03|       |
| 25        | 35.377           | 0.07 | 2.01|       | 47.444           | 0.34 | 2.03|       |
| 26        | 35.383           | 0.07 | 2.00|       | 47.450           | 0.34 | 2.03|       |
| 27        | 35.388           | 0.07 | 2.00|       | 47.456           | 0.34 | 2.02|       |
| 28        | 35.393           | 0.07 | 2.00|       | 47.461           | 0.34 | 2.02|       |
| 29        | 35.397           | 0.07 | 2.00|       | 47.465           | 0.34 | 2.02|       |
| 30        | 35.401           | 0.07 | 2.00|       | 47.469           | 0.34 | 2.02|       |
| 31        | 35.405           | 0.07 | 2.00|       | 47.473           | 0.34 | 2.02|       |
| 32        | 35.408           | 0.07 | 2.00|       | 47.476           | 0.34 | 2.02|       |
| 33        | 35.411           | 0.07 | 2.00|       | 47.479           | 0.34 | 2.02|       |
| 34        | 35.413           | 0.07 | 2.00|       | 47.482           | 0.34 | 2.02|       |
| 35        | 35.416           | 0.07 | 2.00|       | 47.484           | 0.34 | 2.02|       |
| 36        | 35.418           | 0.07 | 2.00|       | 47.487           | 0.34 | 2.02|       |
| 37        | 35.420           | 0.07 | 2.00|       | 47.489           | 0.34 | 2.02|       |
| 38        | 35.422           | 0.07 | 2.00|       | 47.491           | 0.34 | 2.02|       |
| 39        | 35.424           | 0.07 | 2.00|       | 47.492           | 0.34 | 2.02|       |
| 40        | 35.424           | 0.07 | 2.00|       |                     |     |     |       |
| …         | 35.458           | 2.00 |     |       | 47.527           | 2.00|     |       |

Table 3: Comparison of the calculated energies(in eV)of the \(2s^22p^2(1D)nd^2P\) and \(2s^22p^2(1D)ns^2D\) relative to the \(^3P^\ast\) Metastable state of \(\text{O}^+\) with the experimental data of Aguilar et al. [9] and with the recenttheoretical data of Sow et al. [17].

| \(n\) | \(2s^22p^2(1D)nd^2P\) | Diff (%) | \(2s^22p^2(1D)ns^2D\) | Diff (%) |
|-------|------------------|---------|------------------|---------|
|       | Energies | Exp theory | Energies | Exp theory |
|      | SCUNC | ALS | MOAT | SCUNC | ALS | MOAT |
| 5     | 30.393 | 30.393 | 30.393 | 0.00 | 0.00 |       |
| 6     | 31.079 | 31.081 | 31.081 | 0.01 | 0.01 |       |
|       | 30.578 | 30.578 | 30.578 | 0.00 | 0.00 |       |
Comparison of the calculated energies (in eV) of the $2s^22p^3(3S)nd^2D$ and $2s2p^5(3P)np^2D$ relative to the $2p^3(3P)$ state of O+ with the experimental data of Aguilar et al. [9] and with the recent theoretical data of Sow et al. [17].

| n  | $2s^22p^3(3S)nd^2D$ | $2s2p^5(3P)np^2D$ |
|----|---------------------|---------------------|
|    | SCUNC | ALS | MOAT | SCUNC | ALS | MOAT | SCUNC | ALS | MOAT | SCUNC | ALS | MOAT |
| 3  | 31.924 | 31.924 | 31.924 | 39.478 | 39.478 | 39.478 | 0.00 | 0.00 |
| 4  | 33.217 | 33.217 | 33.217 | 43.911 | 43.115 | 43.115 | 0.64 | 0.64 |
| 5  | 33.910 | 33.910 | 33.910 | 45.093 | 45.093 | 45.093 | 0.21 | 0.20 |
| 6  | 34.593 | 34.597 | 34.599 | 46.999 | 46.788 | 0.40 | 0.40 |
| 7  | 34.776 | 34.782 | 34.782 | 46.801 | 46.971 | 0.36 | 0.36 |
| 8  | 34.906 | 34.909 | 34.912 | 46.944 | 47.095 | 0.32 | 0.32 |
| 9  | 35.003 | 35.008 | 35.012 | 47.048 | 47.181 | 0.28 | 0.28 |
| 10 | 35.076 | 35.082 | 35.088 | 47.127 | 47.244 | 0.25 | 0.25 |
| 11 | 35.133 | 35.145 | 35.147 | 47.188 | 47.292 | 0.22 | 0.22 |
| 12 | 35.178 | 35.183 | 35.185 | 47.236 | 47.328 | 0.20 | 0.20 |
| 13 | 35.214 | 35.219 | 35.222 | 47.274 | 47.357 | 0.18 | 0.18 |
| 14 | 35.244 | 35.244 | 35.244 | 47.305 | 47.380 | 0.16 | 0.16 |
| 15 | 35.268 | 35.268 | 35.268 | 47.331 | 47.398 | 0.14 | 0.14 |
| 16 | 35.289 | 35.289 | 35.289 | 47.353 | 47.412 | 0.13 | 0.13 |
| 17 | 35.306 | 35.306 | 35.306 | 47.371 | 47.425 | 0.11 | 0.11 |
SCUNC, Screening constant by unit nuclear charge, present results.
ALS, Advanced Light Source (ALS) of Aguilar et al. [9]
MOAT, Modified Orbital Atomic Theory of Sow et al. [17]

Diff, relative difference: \( \text{Diff} = \frac{|E_{\text{SCUNC}} - E|}{E} \)

**Summary and Conclusion**:

The Screening Constant by Unit Nuclear Charge (SCUNC) method has been applied to report photoionization calculations on the Nitrogen–like O\(^+\) ion. Resonance energies of the \(2s^22p^2(^1D)ns^2D\), \(2s^22p^2(^1D)nd^2P\), \(2s^22p^2(^3D)ns^2S\), \(2s^22p^2(^1S)nd^2D\) and \(2s^2p^3(^3P)np^2D\) Rydberg series from the \(^3\)P\(_{\text{metastable}}\) state of O\(^+\) ion up to \(n = 40\) are reported in this article using the SCUNC method. To analyze our results, the quantum defect \(\delta\) as well as the effective charge \(Z^*\) were calculated. On the whole, good agreements with the experimental and theoretical data are obtained.

It should be mentioned despite its simplicity where the studied resonance energies are calculated using a single analytical formula, the SCUNC formalism provides new high-lying accurate resonance energies. These data may be benchmarked values for future experimental and theoretical studies on this type of ion for the diagnosis of astrophysical and laboratory plasmas. In addition, the very good results obtained in this work points out the possibilities to use the SCUNC formalism in the investigation of high lying Rydberg series of ions containing several electrons.

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