Photoionization of Aluminum-Like $\text{P}^{2+}$ and Magnesium-Like $\text{P}^{3+}$ by the Screening Constant by Unit Nuclear Charge Method

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Abstract: In the present work, accurate high lying single photoionization resonance energies for Aluminium-like $\text{P}^{2+}$ and magnesium-like $\text{P}^{3+}$ are reported. Calculations are performed in the framework of the Screening Constant by Unit Nuclear Charge (SCUNC) formalism. The resonance energies and quantum defects obtained compared very well with experimental data of Hernández et al., (2015) along with DARC, Dirac Atomic R-matrix Codes computations of Wang et al., (2016). Analysis of the present results is achieved in the framework of the standard quantum-defect theory and of the SCUNC-procedure based on the calculation of the effective charge. It is demonstrated that the SCUNC-method can be used to assist fruitfully experiments for identifying narrow resonance energies due to overlapping peaks. New precise data for Aluminium-like $\text{P}^{2+}$ and magnesium-like $\text{P}^{3+}$ ions are presented as useful guidelines for investigators focusing their challenge on the Photoionization of Aluminium-like $\text{P}^{2+}$ and magnesium-like $\text{P}^{3+}$ heavy charged ions in connection with their application in laboratory, astrophysics, and plasma physics. In addition, our predicted data up to $n = 30$ may be of great importance for the atomic physics community in connection with the determination of accurate abundances for phosphorus in the solar photosphere, in solar twins, in the infrared spectrum of Messier 77 galaxy (NGC1068).

Keywords: Photoionization, Resonance Energies, Rydberg Series, Ground State, Metastable State, SCUNC

1. Introduction

Phosphorus is a primary element in the ribonucleic acid (RNA) of all living cells and functions in signal passing for DNA. However, its detection has been difficult in comparison with other basic elements of life, such as carbon, oxygen, etc. Recently, it has been detected in a number of astronomical objects, e.g. in damp galaxies by Molaro et al., 2001 [1] and Welsh et al., 2001 [2]. In addition Caffau and collaborators [3] proposed the possibility that phosphorus could be formed in late stages of stars. Later, Bon-chul et al., 2013 [4] found evidence of phosphorus in supernovae by measuring the infrared spectra in the remnants of Cassiopea A. Extragalactic phosphorus has been observed in the solar photosphere by Caffau et al., 2007 [5], in solar twins by Meléndez et al., 2009 [6], in the infrared spectrum of Messier 77 galaxy (NGC1068) by Oliva et al., 2001 [7] and in globular clusters by Hubrig et al., 2009 [8] thus the determination of observed phosphorus abundances remains an important issue. In a recent past, Hernández et al., 2015 [9] measured the single PI cross sections of Al-like $\text{P}^{2+}$ and Mg-like $\text{P}^{3+}$ based on the merged-beams technique [10] and obtained the resonance energies and quantum defects for the assigned Rydberg series. Very recently the theoretical photoionization of the ground and metastable states $\text{P}^{2+}$ are first time presented in the photon energy range of 30–43.5 eV.
by Wang et al., 2016 [11]. However it should be recalled that, the theoretical PI studies of Al-like P$^{3+}$ are really rare, and there is no corresponding theoretical data in the previous reports and the comprehensive databases, such as the Opacity Project TOPbase [12]. Therefore, to benchmark the PI measurement of experiment for Al-like P$^{3+}$ [9], the theoretical PI cross sections of Al-like P$^{3+}$ are necessary, and the theoretical study can serve as a candidate for the database mentioned above. Moreover, the relative population of ground and metastable states need to be taken into account for determining the absolute PI cross sections. The motivation of this work is to use the screening constant by unit nuclear charge (SCUNC) formalism (Sakho [13–16]; Badiane et al. [18]; Khatri et al [19]) to report accurate high lying Photoionization data for aluminum-like P$^{3+}$ and magnesium-like P$^{3+}$. 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 experimental of Hernández et al., 2015 [9] and theoretical of Wang et al., 2016 [11] data. 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+1L$^\pi$) excited states is expressed in the form (in Rydbergs).

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

(1)

quantum numbers of the (2S+1L)$nl$ Rydberg series used in the empirical determination of the f-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

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

(4)

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

In Eq.(2), $q$ stands for the number of terms in the expansion of the $\beta$-parameter. Generally, precise resonance energies are obtained for $q<5$. The resonance energy are the in the form

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

(5)

In this equation, $R$ is the Rydberg constant, $E_\infty$ denotes the converging limit, $Z_{core}$ represents the electric charge of the $Z_{core}$ 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

$$E_n = E_\infty - \frac{Z_{core}^2}{n^2}$$

(7)

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

$$E_n = E_\infty - \frac{Z_{core}^2}{n^2}$$

(8)
\[ Z^* = \frac{Z_{\text{core}}}{\left(1 - \frac{\delta}{n}\right)} \]  

(8)

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

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

(9)

\[ \lim_{n \to \infty} Z^* = Z_{\text{core}} \]

Besides, comparing Eq.(5) and Eq.(7), the effective charge is in the form

\[ Z^* \approx Z_{\text{core}} \quad \text{if} \quad \delta \geq 0 \]

\[ Z^* \approx Z_{\text{core}} \quad \text{if} \quad \delta \leq 0 \]

(10)

Besides, the \( f_2 \)-parameter in eq.(2) can be theoretically determined from eq.(10) by neglecting the corrective term with the condition

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

(11)

We get then \( f_2 = Z - Z_{\text{core}} \), where \( Z_{\text{core}} \) is deduced from the photoionization process of the considered atomic X\(^{m+} \) system, \( h\nu + X^{m+} \rightarrow X^{(m+j)^+} + e^- \) find then \( Z_{\text{core}} = m+1 \). As an illustration for \( P^{3+} \) we have \( h\nu + P^{3+} \rightarrow P^{4+} + e^- \) from where \( Z_{\text{core}} = 3 \) and for \( P^{4+} \) we have \( h\nu + P^{4+} \rightarrow P^{5+} + e^- \) from where \( Z_{\text{core}} = 4 \). So, for the \( P^{2+} \) ion, \( f_2 = (15-3) = 12.0 \) and for \( P^{3+} \) ion, \( f_2 = (15-4) = 11.0 \). The remaining \( f_1 \)-parameter is to be evaluated empirically using the experimental data of Hernández et al., 2015 [9] for a given \((2^s+1)l_n \) level with \( \nu = 0 \) in Eq.(5). The empirical procedure of the determination of the \( f_1 \)-screening constant along with the corresponding uncertainty have been explained in details in our previous works (Sakho [13–16]; Ba et al. [17]; Badiane et al. [18]). The results obtained are quoted in Tables 1-4.

2.2. Resonance Energies of the 3s3pnp \( ^1P_0, ^3P_1 \), 3s3dnd \( ^1D_2 \) and 3pndn \( ^1D_2 \) Rydberg Series of Aluminium-Like \( P^{3+} \)

The resonance energies for the different Rydberg series studied for the \( P^{3+} \) ion are given by (in Rydberg).

i. For the Rydberg serie 3s3pnp \( ^1P_1 \) originating from the ground state 3s\(^2\)3p\(^2\)(\( ^1P_{1/2} \))

\[ E_n = E_{\infty} - \frac{Z^2}{n^2} \left[ 1 - \frac{f_1^{(1P_0, 2P_{1/2})}}{Z(n-1)} - \frac{f_2^{(3P_0, 2P_{1/2})}}{Z} + \frac{f_1^{(3P_0, 2P_{1/2})}(n-1)}{Z^2(n-2)} \right] \]

(12)

ii. For the Rydberg serie 3s3pnp \( ^3P_1 \) originating from the ground state 3s\(^2\)3p\(^2\)(\( ^3P_{1/2} \))

\[ E_n = E_{\infty} - \frac{Z^2}{n^2} \left[ 1 - \frac{f_1^{(1P_0, 2P_{1/2})}}{Z(n-1)} + \frac{f_2^{(3P_0, 2P_{1/2})}}{Z} + \frac{f_1^{(3P_0, 2P_{1/2})}(n-1)}{Z^2(n-2)} \right] \]

(13)

iii. For the Rydberg serie 3s3pnp \( ^3P_0 \) originating from the metastable state 3s\(^2\)3p\(^2\)(\( ^3P_{3/2} \))

\[ E_n = E_{\infty} - \frac{Z^2}{n^2} \left[ 1 - \frac{f_1^{(1P_0, 2P_{3/2})}}{Z(n-1)} - \frac{f_2^{(3P_0, 2P_{3/2})}}{Z} - \frac{f_1^{(3P_0, 2P_{3/2})}(n-1)}{Z^2(n-2)} \right] \]

(14)

iv. For the Rydberg serie 3s3pnp \( ^1P_1 \) originating from the metastable state 3s\(^2\)3p\(^2\)(\( ^3P_{3/2} \))

\[ E_n = E_{\infty} - \frac{Z^2}{n^2} \left[ 1 - \frac{f_1^{(1P_0, 2P_{3/2})}}{Z(n-1)} - \frac{f_2^{(3P_0, 2P_{3/2})}}{Z} - \frac{f_1^{(3P_0, 2P_{3/2})}(n-1)}{Z^2(n-2)} \right] \]

(15)

v. For the Rydberg serie 3s3dnd \( ^1D_2 \) originating from the metastable state 3s\(^2\)3p\(^2\)(\( ^3P_{3/2} \))


\[ E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - f_1(1D_2, 2^2P_{3/2}) \frac{Z(n-1)}{Z} - f_2(1D_2, 2^2P_{3/2}) \frac{Z}{Z} - f_1(1D_2, 2^2P_{5/2}) \frac{(n-v)}{Z^2(n-v-s^2)(n-v+2s+1)} \right\}^2 \]  

(16)

vi. For the Rydberg serie 3s3dnd \(^1\)D\(_2\) originating from the ground state 3s\(^3\)3p\(^2\)(P\(_{1/2}\))

\[ E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - f_1(1D_2, 2^2P_{1/2}) \frac{Z(n-1)}{Z} - f_2(1D_2, 2^2P_{1/2}) \frac{Z}{Z} - f_1(1D_2, 2^2P_{3/2}) \frac{(n-v)}{Z^2(n-v-s^2)(n-v+2s+1)} \right\}^2 \]  

(17)

vii. For the Rydberg serie 3p\(^3\)nd \(^1\)D\(_2\) originating from initially long-lived metastable P\(^{2+}\) in state term

\[ E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - f_1(3P_0, 2^2P_{1/2}) \frac{Z(n-1)}{Z} - f_2(3P_0, 2^2P_{1/2}) \frac{Z}{Z} - f_1(3P_0, 2^2P_{3/2}) \frac{(n-v)}{Z^2(n-v-s^2)(n-v+2s+1)} \right\}^2 \]  

(18)

2.3. Resonance Energies of the 2p\(^6\)3p\(^n\)p\(^{\ell}\) Rydberg Serie of Magnesium-Like P\(^{3+}\)

Using Eq(5), we obtain the following expressions of the resonance energies for Rydberg series of the ion P\(^{3+}\) (in Rydberg).

i. For the Rydberg serie 2p\(^6\)3p\(^{\ell}\)P\(_{1/2}\) originating from the excited state 2p\(^6\)3s3p\(^{/}\)P\(_0\) of P\(^{3+}\)

\[ E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - f_1(3P_0, 2^2P_{1/2}) \frac{Z(n-1)}{Z} - f_2(3P_0, 2^2P_{1/2}) \frac{Z}{Z} - f_1(3P_0, 2^2P_{3/2}) \frac{(n-v)}{Z^2(n-v-s^2)(n-v+2s+1)} \right\}^2 \]  

(19)

ii. For the Rydberg serie 2p\(^6\)3p\(^{\ell}\)P\(_{1/2}\) originating from the excited state 2p\(^6\)3s3p\(^{2}\)P\(_{2}\) of P\(^{3+}\)

\[ E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - f_1(3P_0, 2^2P_{1/2}) \frac{Z(n-1)}{Z} - f_2(3P_0, 2^2P_{1/2}) \frac{Z}{Z} - f_1(3P_0, 2^2P_{3/2}) \frac{(n-v)}{Z^2(n-v-s^2)(n-v+2s+1)} \right\}^2 \]  

(20)

iii. For the Rydberg serie 2p\(^6\)3p\(^{\ell}\)P\(_{1/2}\) originating from the ground state 2p\(^6\)3s\(^1\)S\(_0\) of P\(^{3+}\)

\[ E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - f_1(3S_0, 2^2P_{1/2}) \frac{Z(n-1)}{Z} - f_2(3S_0, 2^2P_{1/2}) \frac{Z}{Z} - f_1(3S_0, 2^2P_{3/2}) \frac{(n-v)}{Z^2(n-v-s^2)(n-v+2s+1)} \right\}^2 \]  

(21)

In these expressions, \(\nu\) denotes the principal quantum numbers of \((20+2)_{\text{L}0}\) Rydberg series used in the empirical determination of \(f_i\) screening constant. The principle of determining the screening constant \(f_i\) is described in the appendix.

3. Results and Discussion

The results obtained in the present work are tabulated in Tables 1-4. Tables 5-11 lists the resonance energies and quantum defects are obtained, where a comparison between the theoretical and experimental data is made. The analysis of the calculated energy values is made on the basis of the general expression

\[ \delta = n - Z_{\text{core}} \sqrt{\frac{R}{E_\infty - E_n}} \]

of the quantum defect and on the SCUNC analysis conditions (9) recommended by the present formalism. We recall these expressions:

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

For resonance energies the present SCUNC calculations quoted in Tables 1-4 agree well with both the experimental data of Hernandez et al., 2015 [9] and the theoretical calculations from R-matrix of Wang et al., 2016 [11] for \(n = 3–16\) for all the Rydberg series studied as shown in Tables 5-11. These agreements allow one to expect the SCUNC data quoted in Tables 1-4 to be accurate up to \(n = 30\) with a quantum defect almost constant along the series investigated.
In addition the excellent agreement between the experimental measurements along with the R-matrix approach and the SCUNC predictions may demonstrate the accuracy of our results quoted Tables 1-4 where the quantum defect is seen to be quite constant along each series. Is should be mentioned that, the SCUNC conditions analysis (9) are well verified as shown by the data listed in Tables 1-4 for the different Rydberg series studied for aluminum-like P\(^{2+}\) and magnesium-like P\(^{3+}\). It is demonstrated in this work that the SCUNC-method can be used to assist fruitfully experiments for identifying narrow resonance energies due to overlapping peaks. New high lying accurate resonance energies (n = 3–30) are tabulated as benchmarked data for the atomic physics community in connection with the modeling of plasma and astrophysical systems.

| n  | 3s\(^3\)p(\(^2\)P\(_{2/2}\))→3s3pnp\(^1\)P\(_{0}\) | 3s\(^3\)p(\(^2\)P\(_{3/2}\))→3s3pnp\(^1\)P\(_{1}\) |
|----|-------------------------------------------------|-------------------------------------------------|
| 3  | -                                               | -                                               |
| 4  | -                                               | -                                               |
| 5  | -                                               | -                                               |
| 6  | 35.451                                          | -0.21                                           |
| 7  | 36.278                                          | -0.23                                           |
| 8  | 36.818                                          | -0.24                                           |
| 9  | 37.191                                          | -0.25                                           |
| 10 | 37.458                                          | -0.25                                           |
| 11 | 37.657                                          | -0.26                                           |
| 12 | 37.809                                          | -0.26                                           |
| 13 | 37.928                                          | -0.27                                           |
| 14 | 38.022                                          | -0.27                                           |
| 15 | 38.098                                          | -0.28                                           |
| 16 | 38.161                                          | -0.28                                           |
| 17 | 38.213                                          | -0.28                                           |
| 18 | 38.257                                          | -0.29                                           |
| 19 | 38.294                                          | -0.29                                           |
| 20 | 38.326                                          | -0.29                                           |
| 21 | 38.353                                          | -0.29                                           |
| 22 | 38.377                                          | -0.29                                           |
| 23 | 38.397                                          | -0.29                                           |
| 24 | 38.416                                          | -0.30                                           |
| 25 | 38.432                                          | -0.30                                           |
| 26 | 38.446                                          | -0.30                                           |
| 27 | 38.459                                          | -0.30                                           |
| 28 | 38.470                                          | -0.30                                           |
| 29 | 38.480                                          | -0.30                                           |
| 30 | 38.490                                          | -0.30                                           |
| ...| ...                                             | ...                                             |
| ∞  | 38.623\(^*\)                                    | 3.000                                           |

\(^*\)Limits were derived from reference values given by NIST[20].

| n  | 3s\(^3\)p(\(^2\)P\(_{3/2}\))→3s3pnp\(^1\)P\(_{0}\) | 3s\(^3\)p(\(^2\)P\(_{2/2}\))→3s3pnp\(^1\)P\(_{1}\) |
|----|-------------------------------------------------|-------------------------------------------------|
| 3  | -                                               | -                                               |
| 4  | 31.617                                          | -0.20                                           |
| 5  | 34.002                                          | -0.19                                           |
| 6  | 35.346                                          | -0.18                                           |
| 7  | 36.174                                          | -0.17                                           |
| 8  | 36.719                                          | -0.17                                           |
| 9  | 37.097                                          | -0.17                                           |
| 10 | 37.369                                          | -0.16                                           |
| 11 | 37.571                                          | -0.16                                           |
| 12 | 37.726                                          | -0.16                                           |
| 13 | 37.847                                          | -0.16                                           |
| 14 | 37.943                                          | -0.16                                           |
| 15 | 38.021                                          | -0.16                                           |
| 16 | 38.085                                          | -0.16                                           |
| 17 | 38.138                                          | -0.16                                           |
| 18 | 38.183                                          | -0.16                                           |
| 19 | 38.220                                          | -0.16                                           |
| 20 | 38.253                                          | -0.16                                           |
| 21 | 38.280                                          | -0.16                                           |
Table 4. Present calculations of resonance energies ($E_n$eV), quantum defect ($\delta$) and effective charge ($Z^*$) of the 3s3p$^2$ 1S\textsubscript{0} series of the Mg-like $P^{II}$.

| n   | $E_n$ | $\delta$ | $Z^*$ | $E_n$ | $\delta$ | $Z^*$ | $E_n$ | $\delta$ | $Z^*$ |
|-----|-------|----------|-------|-------|----------|-------|-------|----------|-------|
| 5   | 55.064 | 0.15    | 3.036  | 57.032 | 0.15    | 3.036  | 59.000 | 0.15    | 3.036 |
| 26  | 60.000 | 0.15    | 3.036  | 62.000 | 0.15    | 3.036  | 64.000 | 0.15    | 3.036 |
| 27  | 61.000 | 0.15    | 3.036  | 63.000 | 0.15    | 3.036  | 65.000 | 0.15    | 3.036 |
| 28  | 62.000 | 0.15    | 3.036  | 64.000 | 0.15    | 3.036  | 66.000 | 0.15    | 3.036 |
| 29  | 63.000 | 0.15    | 3.036  | 65.000 | 0.15    | 3.036  | 67.000 | 0.15    | 3.036 |
| 30  | 64.000 | 0.15    | 3.036  | 66.000 | 0.15    | 3.036  | 68.000 | 0.15    | 3.036 |
| ... | ...   | ...     | ...   | ...   | ...     | ...   | ...   | ...     | ...   |
| $\infty$ | 57.305 | 0.15    | 3.036  | ...   | ...     | ...   | ...   | ...     | ...   |

*Limits were derived from reference values given by NIST[20].
Comparison of the present SCUNC calculations of resonance energies ($E_{\text{R-matrix}}$, eV) and quantum defect ($\delta$) of the Rydberg series $3s3p^2P^0 \nu$ originating from the ground state $3s^23p^2P^{0}$ with the $R$-matrix calculations of Wang et al., 2016 [11] and with the recent experimental data of Hernández et al., 2015 [9]. $\Delta E_{\text{nuc}}$ denotes the energy difference between the present SCUNC calculations and the experimental data of Hernández et al., 2015.

| n | $3s3p^2P^0\nu \rightarrow 3s3pnp^2P^0_{\nu}$ | SCUNC | R-matrix | Exp. | $\Delta E_{\text{nuc}}$ | $\delta$ | $\delta$ | $\delta$ |
|---|---|---|---|---|---|---|---|---|
| 3 | - | 31.4024 | - | - | - | - | - | - |
| 4 | - | 33.8996 | - | - | - | - | - | - |
| 5 | - | - | - | - | - | - | - | - |
| 6 | 35.451 | 35.451 | 0.000 | -0.21 | - | - | - | - |
| 7 | 36.278 | 36.272 | 0.006 | -0.23 | - | - | - | - |
| 8 | 36.818 | 36.816 | 0.002 | -0.24 | - | - | - | - |
| 9 | 37.191 | 37.184 | 0.007 | -0.25 | - | - | - | - |
| 10 | 37.458 | 37.459 | 0.001 | -0.25 | - | - | - | - |
| 11 | 37.657 | 37.658 | 0.001 | -0.26 | - | - | - | - |
| 12 | 37.809 | 37.811 | 0.002 | -0.26 | - | - | - | - |
| 13 | 37.928 | 37.933 | 0.005 | -0.27 | - | - | - | - |
| 14 | 38.022 | 38.030 | 0.008 | -0.27 | - | - | - | - |
| 15 | 38.098 | 38.107 | 0.009 | -0.28 | - | - | - | - |
| 16 | 38.161 | 38.171 | 0.010 | -0.28 | - | - | - | - |
| ... | ... | ... | ... | ... | ... | ... | ... | ... |
| $\infty$ | 38.623 | 38.4227 | 38.623 | | | | | |

Comparison of the present SCUNC calculations of resonance energies ($E_{\text{R-matrix}}$, eV) and quantum defect ($\delta$) of the Rydberg series $3s3p^2P^0 \nu$ originating from the ground state $3s^23p^2P^{0}$ with the $R$-matrix calculations of Wang et al., 2016 [11] and with the recent experimental data of Hernández et al., 2015 [9]. $\Delta E_{\text{nuc}}$ denotes the energy difference between the present SCUNC calculations and the experimental data of Hernández et al., 2015.

| n | $3s3p^2P^0\nu \rightarrow 3s3pnp^2P^0_{\nu}$ | SCUNC | R-matrix | Exp. | $\Delta E_{\text{nuc}}$ | $\delta$ | $\delta$ | $\delta$ |
|---|---|---|---|---|---|---|---|---|
| 3 | 30.411 | 30.692 | 30.411 | 0.000 | -0.09 | - | - | - |
| 4 | 35.949 | 36.224 | (35.948) | 0.001 | -0.10 | - | - | - |
| 5 | 38.463 | 38.794 | 38.467 | 0.004 | -0.06 | - | - | - |
| 6 | 39.912 | 40.110 | 39.906 | 0.006 | -0.06 | - | - | - |
| 7 | 40.788 | 41.060 | 40.727 | 0.061 | -0.06 | - | - | - |
| 8 | 41.359 | 41.620 | (41.330) | 0.029 | -0.06 | - | - | - |
| 9 | 41.752 | 41.983 | (41.717) | 0.035 | -0.06 | - | - | - |
| 10 | 42.034 | 42.248 | (41.983) | 0.051 | -0.06 | - | - | - |
| 11 | 42.243 | 42.432 | (42.183) | 0.060 | -0.06 | - | - | - |
| ... | ... | ... | ... | ... | ... | ... | ... | ... |
| $\infty$ | 43.244 | 43.5168 | 43.244 | | | | | |
from the metastable state \(3s\,3p^2\,^1P_1\) of \(P^+\) with the R-matrix calculations of Wang et al., 2016 [11] and with the recent experimental data of Hernández et al., 2015 [9]. \(\Delta E_n\) denotes the energy difference between the present SCUNC calculations and the experimental data of Hernández et al., 2015.

### Table 8. Comparison of the present SCUNC calculations of resonance energies (\(E_n\,eV\)) and quantum defect (\(\delta\)) of the Rydberg serie \(3s3p^\nu P_1\) originating from the metastable state \(3s\,3p^2\,^1P_1\) of \(P^+\) with the R-matrix calculations of Wang et al., 2016 [11] and with the recent experimental data of Hernández et al., 2015 [9]. \(\Delta E_n\) denotes the energy difference between the present SCUNC calculations and the experimental data of Hernández et al., 2015.

| \(n\) | \(3s3p^2\,^1P_1\) | \(3s3p^\nu P_1\) |
|---|---|---|
| | SCUNC | R-matrix | Exp. |
| \(E_n\) | \(E_n\) | \(E_n\) | \(\Delta E_n\) | \(\delta\) | \(\delta\) |
| 3 | 30.471 | 30.652 | (30.471) | 0.000 | -0.10 | -0.094 | (-0.10) |
| 4 | 35.957 | 36.224 | (35.948) | 0.009 | -0.12 | -0.117 | (-0.12) |
| 5 | 38.532 | 38.725 | 38.54 | 0.009 | -0.14 | -0.092 | (-0.14) |
| 6 | 39.941 | 40.140 | (39.986) | 0.045 | -0.15 | -0.085 | (-0.20) |
| 7 | 40.794 | 40.980 | 40.789 | 0.005 | -0.17 | -0.046 | -0.16 |
| ... | ... | ... | ... | ... | ... | ... | ... |
| \(\infty\) | 43.175 | 43.4688 | 43.175 |

Table 8: Comparison of the present SCUNC calculations of resonance energies (\(E_n\,eV\)) and quantum defect (\(\delta\)) of the Rydberg series \(3s3p^\nu P_1\) of \(P^+\) originating from the metastable state \(3s\,3p^2\,^1P_1\) of \(P^+\) with the R-matrix calculations of Wang et al., 2016 [11] and with the recent experimental data of Hernández et al., 2015 [9]. \(\Delta E_n\) denotes the energy difference between the present SCUNC calculations and the experimental data of Hernández et al., 2015.

### Table 9. Comparison of the present SCUNC calculations of resonance energies (\(E_n\,eV\)) and quantum defect (\(\delta\)) of \(P^+\) for the following Rydberg series. \(\Delta E_n\) denotes the energy difference between the present SCUNC calculations and the experimental data of Hernández et al., 2015 [9].

| \(n\) | \(3s3p^2\,^1P_1\) | \(3s3p^\nu P_1\) |
|---|---|---|
| | SCUNC | R-matrix | Exp. | SCUNC | R-matrix | Exp. |
| \(E_n\) | \(E_n\) | \(E_n\) | \(\Delta E_n\) | \(\delta\) | \(\delta\) | \(\delta\) |
| 4 | 48.962 | (48.962) | 0.000 | 0.17 | (0.21) | 49.188 | (49.188) | 0.000 | 0.13 | (0.13) |
| 5 | 52.038 | (52.037) | 0.001 | 0.18 | (0.18) | 52.191 | (52.191) | 0.000 | 0.14 | (0.14) |
| ... | ... | ... | ... | ... | ... | ... | ... | ... | ... | ... |
| \(\infty\) | 57.305 | 57.305 | 57.374 | 57.374 |

Table 9: Comparison of the present SCUNC calculations of resonance energies (\(E_n\,eV\)) and quantum defect (\(\delta\)) of \(P^+\) for the following Rydberg series. \(\Delta E_n\) denotes the energy difference between the present SCUNC calculations and the experimental data of Hernández et al., 2015 [9].

### Table 10. Comparison of the present SCUNC calculations of resonance energies (\(E_n\,eV\)) and quantum defect (\(\delta\)) of \(P^+\) for the following Rydberg series. \(\Delta E_n\) denotes the energy difference between the present SCUNC calculations and the experimental data of Hernández et al., 2015 [9].

| \(n\) | \(2p^33p^\nu P_1\) | \(2p^33p^2 P^+\) |
|---|---|---|
| | SCUNC | R-matrix | Exp. | SCUNC | R-matrix | Exp. |
| \(E_n\) | \(E_n\) | \(E_n\) | \(\Delta E_n\) | \(\delta\) | \(\delta\) | \(\delta\) |
| 5 | - | - | - | - | - | - |
| 6 | 46.429 | 46.433 | 0.004 | 0.64 | 0.64 | - | - | - | - |
| 7 | 48.636 | 48.621 | 0.015 | 0.64 | 0.65 | - | - | - | - |
| 8 | 50.002 | 49.993 | 0.009 | 0.63 | 0.64 | - | - | - | - |
| 9 | 50.906 | 50.892 | 0.014 | 0.63 | 0.65 | - | - | - | - |
| 10 | 51.535 | 51.541 | 0.006 | 0.63 | (0.61) | 51.664 | 51.664 | 0.000 | 0.19 | 0.20 |
| 11 | 51.991 | 51.993 | 0.002 | 0.63 | (0.62) | 52.049 | 52.043 | 0.006 | 0.24 | 0.25 |
| 12 | 52.331 | 52.329 | 0.002 | 0.63 | (0.64) | 52.348 | 52.336 | 0.012 | 0.26 | (0.31) |
| 13 | 52.593 | 52.587 | 0.006 | 0.63 | (0.65) | 52.593 | 52.587 | 0.006 | 0.23 | (0.26) |
| ... | ... | ... | ... | ... | ... | ... |
| \(\infty\) | 54.015 | 54.015 | 53.928 | 53.928 |
4. Summary and Conclusion

The screening constant by unit nuclear charge (SCUNC) has been applied to the photoionization of the ground and metastable states of aluminum-like P$^{2+}$ and magnesium-like P$^{3+}$. Excellent agreements are obtained between the present predictions and previous studies from Advanced Light Source experiments at Lawrence Berkeley National Laboratory of Hernández et al., 2015 [9] and calculations from Dirac R-matrix method of Wang et al., 2016 [11]. 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. Finally, our predicted data up to matrix-method for locating and determining the properties of abundances for phosphorus in the solar photosphere, in solar twins, in the infrared spectrum of Messier 77 galaxy (NGC1068).

Appendix Detailed Processes to Evaluate Empirically the Screening Constants $f_i$

In the framework of the Screening constant by unit nuclear charge (SCUNC) method, the screening constants $f_i$ are evaluated from experimental values. They are then determined empirically with a certain absolute error linked to the experimental measurement errors. We move on explaining in detail the principle for determining the absolute values, $\Delta f_i$. Within the framework of the SCUNC formalism, the screening constants, $f_i$, are presented as $f_i=f_{i,\text{exp}}+\Delta f_i$. The absolute errors, $\Delta f_i$ are given by Sakho [13].

$$\Delta f_i = \sqrt{\left(f_i - f_{i,\text{exp}}\right)^2 + \left(f_i - f_{i,\text{exp}}\right)^2}$$

In general, the experimental resonance energies are expressed in the form $E_n = E_{\text{exp}} + \Delta E$, with $\Delta E$ the absolute error on the resonance energies. The $f_i$ screening constants are evaluated using the experimental resonance energies for $n=30$ may be of great importance for the atomic physics community in connection with the determination of accurate abundances for phosphorus in the solar photosphere, in solar twins, in the infrared spectrum of Messier 77 galaxy (NGC1068).

Table 11. Comparison of the present SCUNC calculations of resonance energies ($E_n eV$) and quantum defect ($\delta$) of P$^{+}$ for the following Rydberg serie. $\Delta E_{\text{f}}$ denotes the energy difference between the present SCUNC calculations and the experimental data of Hernández et al., 2015 [9].

| n   | 2p$^3$s$^1$(1S$_0$)$\rightarrow$2p$^3$pns$^1$P$_{1/2}$ | SCUNC | Exp. | $|\Delta E_f|$ | SCUNC | Exp. | $\delta$ | $\delta$ |
|-----|--------------------------------------------------|-------|------|-------------|-------|------|----------|----------|
| 5   | 51.983                                           | 51.983| 0.000| 0.44       | 0.44  |
| 6   | 55.360                                           | 55.401| 0.041| 0.45       | 0.44  |
| 7   | 57.355                                           | 57.354| 0.001| 0.45       | 0.46  |
| $\ldots$ | $\ldots$                              | $\ldots$| $\ldots$| $\ldots$  | $\ldots$|
| $\infty$ | 62.435                                         | 62.435|      |            |       |

In the present work, only $f_i$ is to be evaluated as $f_i=12.0$ for P$^{2+}$ and $f_i=11.0$ for P$^{3+}$. In this case, one equation is required to find the value of $f_i$ in Eq.(23) using the following relations for $n=\nu$.

$$\begin{align*}
E^+ &= E_{\text{exp}} + \Delta E \\
E^- &= E_{\text{exp}} - \Delta E
\end{align*}$$

Let us then apply Eq.(24) to evaluate both $f_i$ and $\Delta f_i$ considering for example the Rydberg serie 3s$^3$p$^3$P$_0$ originating from the ground state 3s$^3$p$^3$(P$_{1/2}$) of P$^{2+}$. For these states, the resonance energies are given by Eq.(12) reminded below

$$E_n = E_{\text{exp}} - Z^2 \frac{n^2}{n^2} \left\{ 1 - \frac{f_1^2 P_0^2 P_{1/2}^2}{Z(n-1)} - \frac{f_2^2 P_0^2 P_{1/2}^2}{Z} - \frac{f_1^2 P_0^2 P_{1/2}^2(n-\nu)}{Z(n+\nu+s-2)^2} \right\}$$

For sake of simplification we put $f_1 = f_2 = (P_0^2, P_{1/2}^2)$. The first entry for the Rydberg serie 3s$^3$p$^3$P$_0$ originating from the ground state 3s$^3$p$^3$(P$_{1/2}$) is $n=\nu = 6$. As $Z=15$ the P$^{2+}$ ion, Eq.(12) above takes the form

$$E_6 = E_{\text{exp}} - \frac{15^2}{6^2} \left\{ 1 - \frac{1}{15(6-1)} \right\}^2 \times 13.606 = E_{\text{exp}} - \frac{15^2}{6^2} \left\{ 1 - \frac{12}{75} \right\}^2 \times 13.606$$

$$E_6 = E_{\text{exp}} - \frac{15^2}{6^2} \left\{ 1 - \frac{12}{75} \right\}^2 \times 13.606$$

\[(25)\]
In Table 5 we pull the experimental resonance energy $E_\text{e}(35.451\pm0.035)$eV, $n=\nu=6$ from Hernández et al., 2015 [9] along with the energy limits $E_\infty=38.623$eV. Using Eqs.(24) and (25), we find

$$
\begin{align*}
35.451 &= 38.623 - \frac{15^2}{6^2} \left\{ \frac{1}{75} \frac{12}{15} \right\}^2 \times 13.606 \\
35.451 + 0.035 &= 38.623 - \frac{15^2}{6^2} \left\{ \frac{1}{75} \frac{12}{15} \right\}^2 \times 13.606 \\
35.451 - 0.035 &= 38.623 - \frac{15^2}{6^2} \left\{ \frac{-1}{75} \frac{12}{15} \right\}^2 \times 13.606 
\end{align*}
$$

Simplifying these equations, we get

$$
\begin{align*}
1 - \frac{f_1}{75} = 0.193135161 \\
1 - \frac{f_1^+}{75} = 0.192066674 \\
1 - \frac{f_1^-}{75} = 0.194197769
\end{align*}
\Rightarrow \begin{align*}
f_1 &= 0.514862879 \\
f_1^+ &= 0.594999398 \\
f_1^- &= 0.435167268
\end{align*}
$$

Using the results (26) and Eq.(22), the absolute error, $\Delta f_i$, is equal to

$$
\Delta f_i = \sqrt{\frac{(0.514862879 - 0.594999398)^2 + (0.514862879 - 0.435167268)^2}{2}} = 0.080
$$

The empirical screening constant, $f_1 = f_1(3P_0, 2P_{1/2}) = 0.515$, is then presented as $f_1(3P_0, 2P_{1/2}) = 0.515 \pm 0.080$. The other absolute errors, $\Delta f_i$ for the remaining series are evaluated similarly.

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