

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

Momar Talla Gning^{1,*}, Jean Kouhissoré Badiane², Abdourahmane Diallo², Mamadou Diouldé Ba², Ibrahima Sakho¹

¹Department of Experiential Sciences, UFR Sciences and Technologies, University of Thies, Thies, Senegal

²Department of Physics, UFR Sciences and Technologies, University Assane Seck of Ziguinchor, Ziguinchor, Senegal

Email address:

m.gning20150917@zig.univ.sn (M. T. Gning), j.badiane287@zig.univ.sn (J. K. Badiane), a.diallo1483@zig.univ.sn (A. Diallo), m.ba2664@zig.univ.sn (M. D. Ba), ibrahima.sakho@univ-thies.sn (I. Sakho)

*Corresponding author

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Abstract: In the present work, accurate high lying single photoionization resonance energies for Aluminium-like P^{2+} and magnesium-like 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 P^{2+} and magnesium-like P^{3+} ions are presented as useful guidelines for investigators focusing their challenge on the Photoionization of aluminum-like P^{2+} and magnesium-like 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 P^{2+} and Mg-like 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 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^{2+} 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^{2+} [9], the theoretical PI cross sections of Al-like P^{2+} 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]; Ba *et al.* [17]; Badiane *et al.* [18]; Khatri *et al.* [19]) to report accurate high lying Photoionization data for aluminum-like P^{2+} 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 $(Nl, nl'; {}^{2S+1}L^\pi)$ excited states is expressed in the form (in Rydbergs).

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

In this equation, the principal quantum numbers N and n are respectively for the inner and the outer electron of the helium-isoelectronic series. The β -parameters are screening constants by unit nuclear charge expanded in inverse powers of Z and given by

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

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

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

$$E_n = E_\infty - \frac{Z^2}{n^2} \left[1 - \beta(Z; {}^{2S+1}L_J, n, s, \mu, \nu) \right]^2 \quad (3)$$

In this equation, ν and μ ($\mu > \nu$) denote the principal

$$E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - \frac{f_1({}^{2S+1}L^\pi)}{Z(n-1)} - \frac{f_2({}^{2S+1}L^\pi)}{Z} \pm \sum_{k=1}^q \sum_{k'=1}^{q'} f_1^{k'} F(n, \mu, \nu, s) \times \left(\frac{1}{Z} \right)^k \right\}^2 \quad (5)$$

The quantity

$$\pm \sum_{k=1}^q \sum_{k'=1}^{q'} f_1^{k'} F(n, \mu, \nu, s) \times \left(\frac{1}{Z} \right)^k$$

is a corrective term introduced to stabilize the resonance energies with increasing the principal quantum number n . In general, resonance energies are analyzed from the standard quantum-defect expansion formula

$$E_n = E_\infty - \frac{RZ_{core}^2}{(n-\delta)^2} \quad (6)$$

quantum numbers of the $({}^{2S+1}L_J)nl$ Rydberg series used in the empirical determination of the f_i -screening constants, s represents the spin of the nl -electron ($s = 1/2$), E_∞ is the energy value of the series limit, E_n denotes the resonance energy and Z stands for the atomic number. The β -parameters are screening constants by unit nuclear charge expanded in inverse powers of Z and given by

$$\beta(Z, {}^{2S+1}L_J, n, s, \mu, \nu) = \sum_{k=1}^q f_k \left(\frac{1}{Z} \right)^k \quad (4)$$

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

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

In this equation, R is the Rydberg constant, E_∞ denotes the converging limit, Z_{core} represents the electric charge of the Z_{core} ion, and δ means the quantum defect. In addition, theoretical and measured energy positions can be analyzed by calculating the Z^* effective charge in the framework of the SCUNC-procedure

$$E_n = E_\infty - \frac{Z^{*2}}{n^2} R \quad (7)$$

The relationship between Z^* and δ is in the form

$$Z^* = \frac{Z_{core}}{\left(1 - \frac{\delta}{n}\right)} \quad (8)$$

$$\begin{cases} Z^* \geq Z_{core} & \text{if } \delta \geq 0 \\ Z^* \leq Z_{core} & \text{if } \delta \leq 0 \end{cases} \quad (9)$$

$$\lim_{n \rightarrow \infty} Z^* = Z_{core}$$

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

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

$$Z^* = Z \left\{ 1 - \frac{f_1(2S+1L^\pi)}{Z(n-1)} - \frac{f_2(2S+1L^\pi)}{Z} \pm \sum_{k=1}^q \sum_{k'=1}^{q'} f_1^{k'} F(n, ?, \nu, s) \times \left(\frac{1}{Z}\right)^k \right\} \quad (10)$$

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

$$\lim_{n \rightarrow \infty} Z^* = Z \left(1 - \frac{f_2(2S+1L^\pi)}{Z} \right) = Z_{core} \quad (11)$$

We get then $f_2 = Z - Z_{core}$, where Z_{core} is deduced from the photoionization process of the considered atomic X^{m+} system, $h\nu + X^{m+} \rightarrow X^{(m+1)+} + e^-$ find then $Z_{core} = m+1$. As an illustration for P^{2+} we have $h\nu + P^{2+} \rightarrow P^{3+} + e^-$ from where $Z_{core} = 3$ and for P^{3+} we have $h\nu + P^{3+} \rightarrow P^{4+} + e^-$ from where $Z_{core} = 4$. 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 $(2S+1L_j)nl$ 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 $3s3pnp$ ($^3P_0, ^1P_1$), $3s3dnd$ (1D_2) and $3p^2nd$ (1D_2) Rydberg Series of Aluminium-Like P^{2+}

The resonance energies for the different Rydberg series studied for the P^{2+} ion are given by (in Rydberg).

- i. For the Rydberg series $3s3pnp$ 3P_0 originating from the ground state $3s^23p(^2P_{1/2})$

$$E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - \frac{f_1(^3P_0, ^2P_{1/2})}{Z(n-1)} - \frac{f_2(^3P_0, ^2P_{1/2})}{Z} - \frac{f_1(^3P_0, ^2P_{1/2})(n-\nu)}{Z(n+\nu+2s+7)(n+\nu-3)} + \frac{f_1(^3P_0, ^2P_{1/2})(n-\nu)}{Z^2(n+\nu+s-2)^2} - \frac{f_1(^3P_0, ^2P_{1/2})(n-\nu)}{Z^3(n+\nu+s)(n+\nu+s-1)} \right\}^2 \quad (12)$$

- ii. For the Rydberg series $3s3pnp$ 1P_1 originating from the ground state $3s^23p(^2P_{1/2})$

$$E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - \frac{f_1(^1P_1, ^2P_{1/2})}{Z(n-1)} - \frac{f_2(^1P_1, ^2P_{1/2})}{Z} - \frac{f_1(^1P_1, ^2P_{1/2})(n-\nu)}{Z^2(n-s)(n-\nu-s/2-1)} + \frac{f_1(^1P_1, ^2P_{1/2})(n-\nu)}{Z^3(n+\nu+s-2)^2(n-\nu-s/2-1)} \right\}^2 \quad (13)$$

- iii. For the Rydberg series $3s3pnp$ 3P_0 originating from the metastable state $3s^23p(^2P_{3/2})$

$$E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - \frac{f_1(^3P_0, ^2P_{3/2})}{Z(n-1)} - \frac{f_2(^3P_0, ^2P_{3/2})}{Z} - \frac{f_1(^3P_0, ^2P_{3/2})(n-\nu-1)}{Z^2(n+\nu-s+2)(n+2\nu-2)} \right\}^2 \quad (14)$$

- iv. For the Rydberg series $3s3pnp$ 1P_1 originating from the metastable state $3s^23p(^2P_{3/2})$

$$E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - \frac{f_1(^3P_0, ^2P_{3/2})}{Z(n-1)} - \frac{f_2(^3P_0, ^2P_{3/2})}{Z} - \frac{f_1(^3P_0, ^2P_{3/2})(n-\nu)(\nu+s/2+1)}{Z^2(n+\nu-2s-1)} \right\}^2 \quad (15)$$

- v. For the Rydberg series $3s3dnd$ 1D_2 originating from the metastable state $3s^23p(^2P_{3/2})$

$$E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - \frac{f_1(^1D_2, ^2P_{3/2})}{Z(n-1)} - \frac{f_2(^1D_2, ^2P_{3/2})}{Z} - \frac{f_1(^1D_2, ^2P_{3/2})(n-\nu)}{Z^2(n-\nu-s^2)(n-\nu+2s+1)} \right\}^2 \quad (16)$$

vi. For the Rydberg series $3s3dnd \ ^1D_2$ originating from the ground state $3s^23p(^2P_{1/2})$

$$E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - \frac{f_1(^1D_2, ^2P_{1/2})}{Z(n-1)} - \frac{f_2(^1D_2, ^2P_{1/2})}{Z} - \frac{f_1(^1D_2, ^2P_{1/2})(n-\nu)}{Z^2(n-\nu-s^2)(n-\nu+2s+1)} \right\}^2 \quad (17)$$

vii. For the Rydberg series $3p^2nd \ ^1D_2$ originating from initially long-lived metastable P^{2+} in state term $3s3p^2(^4P_{1/2})$

$$E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - \frac{f_1(^1D_2, ^4P_{1/2})}{Z(n-1)} - \frac{f_2(^1D_2, ^4P_{1/2})}{Z} - \frac{f_1(^1D_2, ^4P_{1/2})(n-\nu)}{Z^2(n+\nu+s+5)(n-\nu+s+1)} \right\}^2 \quad (18)$$

2.3. Resonance Energies of the $2p^63pnp(^2P_{1/2})$ 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 series $2p^63p(^2P_{1/2})np$ originating from the excited state $2p^63s3p(^3P_0)$ of P^{3+}

$$E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - \frac{f_1(^3P_0, ^2P_{1/2})}{Z(n-1)} - \frac{f_2(^3P_0, ^2P_{1/2})}{Z} - \frac{f_1(^3P_0, ^2P_{1/2})(n-\nu-1)}{Z^2(n+\nu-s+1)(n+\nu-1)} \right\}^2 \quad (19)$$

ii. For the Rydberg series $2p^63p(^2P_{1/2})np$ originating from the excited state $2p^63s3p(^3P_2)$ of P^{3+}

$$E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - \frac{f_1(^3P_2, ^2P_{1/2})}{Z(n-1)} - \frac{f_2(^3P_2, ^2P_{1/2})}{Z} - \frac{f_1(^3P_2, ^2P_{1/2})(n-\nu)}{Z^2(n-\nu-s)(n-\nu+2s+4)} - \frac{f_1^2(^3P_2, ^2P_{1/2})(n-\nu)^2}{Z^3(n-\nu-s^2-0,5)(n-\nu-s+1)} \right\}^2 \quad (20)$$

iii. For the Rydberg series $2p^63p(^2P_{1/2})np$ originating from the ground state $2p^63s^2(^1S_0)$ of P^{3+}

$$E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - \frac{f_1(^1S_0, ^2P_{1/2})}{Z(n-1)} - \frac{f_2(^1S_0, ^2P_{1/2})}{Z} - \frac{f_1^2(^1S_0, ^2P_{1/2})(n-\nu)}{Z^2(n-\nu+2s+0,75)^2} - \frac{f_1(^1S_0, ^2P_{1/2})(n-\nu)}{Z^3(n-\nu-s^2-0,5)(n+\nu-s)^2} \right\}^2 \quad (21)$$

In these expressions, ν denotes the principal quantum numbers of $(^{2S+1}L_J)nl$ 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

$$\delta = n - Z_{core} \sqrt{\frac{R}{(E_\infty - E_n)}}$$

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

$$\begin{cases} Z^* \geq Z_{core} & \text{if } \delta \geq 0 \\ Z^* \leq Z_{core} & \text{if } \delta \leq 0 \\ \lim_{n \rightarrow \infty} Z^* = Z_{core} \end{cases}$$

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. It 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.

Table 1. Present calculations of resonance energies (E_n, eV), quantum defect (δ) and effective charge (Z^*) of the $3s3pnp\ ^3P_0$ and $3s3pnp\ ^1P_1$ series of P^{2+} .

n	$3s^23p(^2P_{1/2}) \rightarrow 3s3pnp\ ^3P_0$			$3s^23p(^2P_{1/2}) \rightarrow 3s3pnp\ ^1P_1$		
	$f_1(^3P_0, ^2P_{1/2}) = 0.515 \pm 0.080; \nu=6$			$f_1(^1P_1, ^2P_{1/2}) = 0.173 \pm 0.080; \nu=3$		
	E_n	δ	Z^*	E_n	δ	Z^*
3	-	-	-	30.411	-0.09	2.914
4	-	-	-	35.949	-0.10	2.942
5	-	-	-	38.463	-0.06	2.957
6	35.451	-0.21	2.897	39.912	-0.06	2.965
7	36.278	-0.23	2.914	40.788	-0.06	2.971
8	36.818	-0.24	2.926	41.359	-0.06	2.975
9	37.191	-0.25	2.936	41.752	-0.06	2.978
10	37.458	-0.25	2.943	42.034	-0.06	2.981
11	37.657	-0.26	2.949	42.243	-0.06	2.983
12	37.809	-0.26	2.953	42.402	-0.06	2.984
13	37.928	-0.27	2.957	42.526	-0.06	2.986
14	38.022	-0.27	2.960	42.624	-0.06	2.987
15	38.098	-0.28	2.963	42.704	-0.06	2.988
16	38.161	-0.28	2.966	42.769	-0.06	2.988
17	38.213	-0.28	2.968	42.823	-0.06	2.989
18	38.257	-0.29	2.970	42.868	-0.06	2.990
19	38.294	-0.29	2.971	42.907	-0.06	2.990
20	38.326	-0.29	2.973	42.940	-0.06	2.991
21	38.353	-0.29	2.974	42.968	-0.06	2.991
22	38.377	-0.29	2.975	42.992	-0.06	2.992
23	38.397	-0.29	2.977	43.014	-0.06	2.992
24	38.416	-0.30	2.978	43.032	-0.06	2.992
25	38.432	-0.30	2.979	43.049	-0.06	2.993
26	38.446	-0.30	2.979	43.064	-0.06	2.993
27	38.459	-0.30	2.980	43.077	-0.06	2.993
28	38.470	-0.30	2.981	43.088	-0.06	2.994
29	38.480	-0.30	2.982	43.099	-0.06	2.994
30	38.490	-0.30	2.982	43.108	-0.06	2.994
...
∞	38.623 ^a		3.000	43.244 ^a		3.000

^aLimits were derived from reference values given by NIST[20].

Table 2. Present calculations of resonance energies (E_n, eV), quantum defect (δ) and effective charge (Z^*) of the $3s3pnp\ ^3P_0$ and $3s3pnp\ ^1P_1$ series of P^{2+} .

n	$3s^23p(^2P_{3/2}) \rightarrow 3s3pnp\ ^3P_0$			$3s^23p(^2P_{3/2}) \rightarrow 3s3pnp\ ^1P_1$		
	$f_1(^3P_0, ^2P_{3/2}) = 0.432 \pm 0.080; \nu=4$			$f_1(^1P_1, ^2P_{3/2}) = 0.2022 \pm 0.0800; \nu=4$		
	E_n	δ	Z^*	E_n	δ	Z^*
3	-	-	-	30.471	-0.10	2.899
4	31.617	-0.20	2.856	35.957	-0.12	2.933
5	34.002	-0.19	2.892	38.532	-0.14	2.949
6	35.346	-0.18	2.914	39.941	-0.15	2.960
7	36.174	-0.17	2.928	40.794	-0.17	2.966
8	36.719	-0.17	2.938	41.350	-0.19	2.971
9	37.097	-0.17	2.946	41.731	-0.21	2.975
10	37.369	-0.16	2.952	42.005	-0.23	2.978
11	37.571	-0.16	2.957	42.207	-0.25	2.980
12	37.726	-0.16	2.961	42.361	-0.27	2.982
13	37.847	-0.16	2.964	42.481	-0.29	2.983
14	37.943	-0.16	2.967	42.577	-0.31	2.984
15	38.021	-0.16	2.969	42.654	-0.32	2.986
16	38.085	-0.16	2.971	42.717	-0.34	2.987
17	38.138	-0.16	2.973	42.769	-0.36	2.987
18	38.183	-0.16	2.975	42.813	-0.38	2.988
19	38.220	-0.16	2.976	42.850	-0.40	2.989
20	38.253	-0.16	2.977	42.881	-0.42	2.989
21	38.280	-0.16	2.978	42.909	-0.44	2.990

n	$3s^23p(^2P_{3/2}) \rightarrow 3s3pnp\ ^3P_0$			$3s^23p(^2P_{3/2}) \rightarrow 3s3pnp\ ^1P_1$		
	$f_1(^3P_0, ^2P_{3/2}) = 0.432 \pm 0.080; \nu=4$			$f_1(^1P_1, ^2P_{3/2}) = 0.2022 \pm 0.0800; \nu=4$		
	E_n	δ	Z^*	E_n	δ	Z^*
22	38.305	-0.16	2.979	42.932	-0.46	2.990
23	38.326	-0.16	2.980	42.953	-0.48	2.991
24	38.344	-0.16	2.981	42.971	-0.50	2.991
25	38.360	-0.16	2.982	42.987	-0.52	2.992
26	38.375	-0.16	2.983	43.001	-0.54	2.992
27	38.388	-0.16	2.983	43.014	-0.56	2.992
28	38.400	-0.16	2.984	43.025	-0.58	2.993
29	38.410	-0.16	2.985	43.035	-0.60	2.993
30	38.419	-0.16	2.985	43.044	-0.62	2.993
...
∞	38.554 ^a		3.000	43.175 ^a		3.000

^aLimits were derived from reference values given by NIST[20].

Table 3. Present calculations of resonance energies (E_n, eV), quantum defect (δ) and effective charge (Z^*) of the $3s3dnd\ ^1D_2$ and $3p^2nd\ ^1D_2$ series of P^{2+} .

n	$3s^23p(^2P_{3/2}) \rightarrow 3s3dnd\ ^1D_2$			$3s^23p(^2P_{1/2}) \rightarrow 3s3dnd\ ^1D_2$			$3s3p^2(^4P_{1/2}) \rightarrow 3p^2nd\ ^1D_2$		
	$f_1(^1D_2, ^2P_{3/2}) = -0.397 \pm 0.080; \nu=4$			$f_1(^1D_2, ^2P_{1/2}) = -0.308 \pm 0.080; \nu=4$			$f_1(^1D_2, ^4P_{1/2}) = -2.838 \pm 0.080; \nu=4$		
	E_n	δ	Z^*	E_n	δ	Z^*	E_n	δ	Z^*
4	48.962	0.17	3.132	49.188	0.13	3.103	29.512	0.96	3.946
5	52.038	0.18	3.099	52.191	0.14	3.077	35.242	0.96	3.709
6	53.704	0.17	3.079	53.818	0.13	3.062	37.923	0.96	3.568
7	54.685	0.16	3.066	54.781	0.13	3.051	39.388	0.97	3.473
8	55.313	0.16	3.057	55.399	0.13	3.044	40.275	0.97	3.405
9	55.739	0.16	3.050	55.820	0.12	3.038	40.853	0.97	3.355
10	56.041	0.16	3.044	56.119	0.12	3.034	41.250	0.97	3.315
11	56.264	0.15	3.040	56.339	0.12	3.031	41.534	0.97	3.284
12	56.432	0.15	3.036	56.506	0.12	3.028	41.745	0.98	3.258
13	56.563	0.15	3.033	56.636	0.12	3.026	41.905	0.98	3.236
14	56.667	0.15	3.031	56.739	0.12	3.024	42.030	0.98	3.218
15	56.750	0.15	3.028	56.821	0.12	3.022	42.129	0.98	3.203
16	56.818	0.15	3.026	56.889	0.12	3.021	42.209	0.98	3.189
17	56.874	0.15	3.025	56.944	0.12	3.019	42.275	0.98	3.177
18	56.921	0.15	3.023	56.991	0.12	3.018	42.329	0.98	3.167
19	56.960	0.15	3.022	57.031	0.12	3.017	42.375	0.98	3.158
20	56.994	0.15	3.021	57.064	0.12	3.016	42.413	0.98	3.149
21	57.023	0.15	3.020	57.093	0.11	3.015	42.446	0.98	3.142
22	57.049	0.15	3.019	57.118	0.11	3.015	42.475	0.99	3.135
23	57.071	0.15	3.018	57.140	0.11	3.014	42.499	0.99	3.129
24	57.090	0.15	3.017	57.159	0.11	3.013	42.521	0.99	3.123
25	57.107	0.15	3.017	57.176	0.11	3.013	42.540	0.99	3.118
26	57.122	0.15	3.016	57.191	0.11	3.012	42.556	0.99	3.114
27	57.135	0.15	3.015	57.205	0.11	3.012	42.571	0.99	3.109
28	57.147	0.15	3.015	57.217	0.11	3.011	42.584	0.99	3.105
29	57.158	0.15	3.014	57.227	0.11	3.011	42.596	0.99	3.101
30	57.168	0.15	3.014	57.237	0.11	3.011	42.606	0.99	3.098
...
∞	57.305 ^a		3.000	57.374 ^a		3.000	42.752 ^a		3.000

^aLimits were derived from reference values given by NIST[20].

Table 4. Present calculations of resonance energies (E_n, eV), quantum defect (δ) and effective charge (Z^*) of the $2p^63pnp\ ^2P_{1/2}$ and $2p^63pns\ ^2P_{1/2}$ series of the Mg-like P^{3+} .

n	$2p^63s3p(^3P_0) \rightarrow 2p^63pnp\ ^2P_{1/2}$			$2p^63s3p(^3P_2) \rightarrow 2p^63pnp\ ^2P_{1/2}$			$2p^63s^2(^1S_0) \rightarrow 2p^63pns\ ^2P_{1/2}$		
	$f_1(^3P_0, ^2P_{1/2}) = -2.395 \pm 0.080; \nu=6$			$f_1(^3P_2, ^2P_{1/2}) = -0.713 \pm 0.080; \nu=10$			$f_1(^1S_0, ^2P_{1/2}) = -1.529 \pm 0.080; \nu=5$		
	E_n	δ	Z^*	E_n	δ	Z^*	E_n	δ	Z^*
5	-	-	-	-	-	-	51.983	0.44	4.382
6	46.429	0.64	4.479	-	-	-	55.360	0.45	4.306
7	48.636	0.64	4.399	-	-	-	57.355	0.45	4.255
8	50.002	0.63	4.342	-	-	-	58.614	0.45	4.218
9	50.906	0.63	4.299	-	-	-	59.458	0.45	4.191
10	51.535	0.63	4.266	51.664	0.19	4.143	60.050	0.45	4.170
11	51.991	0.63	4.239	52.049	0.24	4.119	60.481	0.45	4.153
12	52.331	0.63	4.218	52.348	0.26	4.102	60.805	0.44	4.139
13	52.593	0.63	4.200	52.593	0.23	4.089	61.055	0.44	4.127

n	$2p^6 3s3p(^3P_0) \rightarrow 2p^6 3pnp\ ^2P_{1/2}$			$2p^6 3s3p(^3P_2) \rightarrow 2p^6 3pnp\ ^2P_{1/2}$			$2p^6 3s(^1S_0) \rightarrow 2p^6 3pns\ ^2P_{1/2}$		
	$f_1(^3P_0, ^2P_{1/2}) = -2.395 \pm 0.080; \nu=6$			$f_1(^3P_2, ^2P_{1/2}) = -0.713 \pm 0.080; \nu=10$			$f_1(^1S_0, ^2P_{1/2}) = -1.529 \pm 0.080; \nu=5$		
	E_n	δ	Z^*	E_n	δ	Z^*	E_n	δ	Z^*
14	52.797	0.63	4.184	52.781	0.22	4.079	61.251	0.44	4.118
15	52.961	0.63	4.171	52.931	0.22	4.071	61.408	0.44	4.109
16	53.094	0.63	4.160	53.054	0.22	4.065	61.536	0.44	4.102
17	53.203	0.63	4.150	53.155	0.22	4.059	61.641	0.44	4.096
18	53.294	0.63	4.141	53.240	0.22	4.055	61.729	0.44	4.090
19	53.370	0.63	4.133	53.311	0.22	4.051	61.803	0.44	4.085
20	53.435	0.63	4.126	53.372	0.22	4.048	61.866	0.44	4.080
21	53.490	0.63	4.120	53.424	0.22	4.045	61.920	0.43	4.076
22	53.538	0.63	4.114	53.469	0.22	4.042	61.967	0.43	4.073
23	53.580	0.63	4.109	53.509	0.22	4.040	62.008	0.43	4.070
24	53.616	0.63	4.104	53.543	0.22	4.038	62.043	0.43	4.066
25	53.648	0.63	4.100	53.574	0.22	4.036	62.074	0.43	4.064
26	53.677	0.63	4.096	53.601	0.22	4.034	62.102	0.43	4.061
27	53.702	0.63	4.092	53.625	0.22	4.032	62.127	0.43	4.059
28	53.724	0.63	4.089	53.646	0.22	4.031	62.149	0.43	4.057
29	53.745	0.63	4.086	53.665	0.22	4.030	62.168	0.43	4.055
30	53.763	0.63	4.083	53.683	0.22	4.029	62.186	0.43	4.053
...
∞	53.928 ^a		4.000	53.928 ^a		4.000	62.435 ^a		4.000

^aLimits were derived from reference values given by NIST[20].

Table 5. Comparison of the present SCUNC calculations of resonance energies (E_n, eV) and quantum defect (δ) of the Rydberg serie $3s3pnp\ ^3P_0$ originating from the ground state $3s^2 3p(^2P_{1/2})$ of P^{2+} 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	$3s^2 3p(^2P_{1/2}) \rightarrow 3s3pnp\ ^3P_0$						
	SCUNC		R-matrix	Exp.	SCUNC		Exp.
	E_n	E_n	E_n	$ \Delta E_n $	δ	δ	δ
3	-	31.4024	-	-	-	-0.146	-
4	-	33.8096	-	-	-	-0.152	-
5	-	-	-	-	-	-	-
6	35.451	-	35.451	0.000	-0.21	-	-0.21
7	36.278	-	36.272	0.006	-0.23	-	-0.21
8	36.818	-	36.816	0.002	-0.24	-	-0.23
9	37.191	-	37.184	0.007	-0.25	-	-0.22
10	37.458	-	37.459	0.001	-0.25	-	-0.25
11	37.657	-	37.658	0.001	-0.26	-	-0.26
12	37.809	-	37.811	0.002	-0.26	-	-0.28
13	37.928	-	37.933	0.005	-0.27	-	-0.32
14	38.022	-	38.030	0.008	-0.27	-	-0.37
15	38.098	-	38.107	0.009	-0.28	-	-0.41
16	38.161	-	38.171	0.010	-0.28	-	-0.46
...
∞	38.623	38.4227	38.623				

Table 6. Comparison of the present SCUNC calculations of resonance energies (E_n, eV) and quantum defect (δ) of the Rydberg serie $3s3pnp\ ^1P_1$ originating from the ground state $3s^2 3p(^2P_{1/2})$ of P^{2+} 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	$3s^2 3p(^2P_{1/2}) \rightarrow 3s3pnp\ ^1P_1$						
	SCUNC		R-matrix	Exp.	SCUNC		Exp.
	E_n	E_n	E_n	$ \Delta E_n $	δ	δ	δ
3	30.411	30.692	30.411	0.000	-0.09	-0.09	-0.09
4	35.949	36.224	(35.948)	0.001	-0.10	-0.098	(-0.10)
5	38.463	38.794	38.467	0.004	-0.06	-0.09	-0.06
6	39.912	40.110	39.906	0.006	-0.06	-0.047	-0.06
7	40.788	41.060	40.727	0.061	-0.06	-0.06	0.03
8	41.359	41.620	(41.330)	0.029	-0.06	-0.03	(0.01)
9	41.752	41.983	(41.717)	0.035	-0.06	0.06	(0.05)
10	42.034	42.248	(41.983)	0.051	-0.06	0.17	(0.14)
11	42.243	42.432	(42.183)	0.060	-0.06	-0.37	(0.26)
...
∞	43.244	43.5168	43.244				

Table 7. Comparison of the present SCUNC calculations of resonance energies (E_n, eV) and quantum defect (δ) of the Rydberg serie $3s3pnp\ ^3P_0$ originating

from the metastable state $3s^2 3p(^2P_{3/2})$ of P^{2+} 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	$3s^2 3p(^2P_{3/2}) \rightarrow 3s3pnp\ ^3P_0$						
	SCUNC		R-matrix		Exp.		
	E_n	E_n	E_n	$ \Delta E_n $	δ	δ	δ
3	-	-	-	-	-	-	-
4	31.617	-	(31.618)	0.001	-0.20	-	(-0.20)
5	34.002	-	33.983	0.019	-0.19	-	-0.17
6	35.346	-	-	-	-0.18	-	-
7	36.174	-	-	-	-0.17	-	-
8	36.719	-	36.723	0.004	-0.17	-	-0.17
9	37.097	-	37.096	0.001	-0.17	-	-0.16
...	...	-	...	-	-	-	-
∞	38.085	-	38.085	-	-	-	-

Table 8. Comparison of the present SCUNC calculations of resonance energies (E_n , eV) and quantum defect (δ) of the Rydberg serie $3s3pnp\ ^1P_1$ originating from the metastable state $3s^2 3p(^2P_{3/2})$ of P^{2+} 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	$3s^2 3p(^2P_{3/2}) \rightarrow 3s3pnp\ ^1P_1$						
	SCUNC		R-matrix		Exp.		
	E_n	E_n	E_n	$ \Delta E_n $	δ	δ	δ
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	38.541	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
...	-	-	-	-
∞	43.175	43.4688	43.175	-	-	-	-

Table 9. Comparison of the present SCUNC calculations of resonance energies (E_n , eV) and quantum defect (δ) of P^{2+} 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	$3s^2 3p(^2P_{3/2}) \rightarrow 3s3dnd\ ^1D_2$				$3s^2 3p(^2P_{1/2}) \rightarrow 3s3dnd\ ^1D_2$					
	SCUNC		Exp.		SCUNC		Exp.			
	E_n	E_n	$ \Delta E_n $	δ	E_n	E_n	$ \Delta E_n $	δ		
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)
...	-	-	-	-	-	-
∞	57.305	57.305	-	-	-	57.374	57.374	-	-	-

n	$3s3p^2(^4P_{1/2}) \rightarrow 3p^2nd\ ^1D_2$			
	SCUNC		Exp.	
	E_n	E_n	$ \Delta E_n $	δ
4	29.512	(29.512)	0.000	0.96
5	35.242	(35.241)	0.001	0.96
...	-	-
∞	42.752	42.752	-	-

Table 10. Comparison of the present SCUNC calculations of resonance energies (E_n , eV) and quantum defect (δ) of P^{3+} 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	$2p^6 3s3p(^3P_0) \rightarrow 2p^6 3pnp\ ^2P_{1/2}$				$2p^6 3s3p(^3P_2) \rightarrow 2p^6 3pnp\ ^2P_{1/2}$					
	SCUNC		Exp.		SCUNC		Exp.			
	E_n	E_n	$ \Delta E_n $	δ	E_n	E_n	$ \Delta E_n $	δ		
5	-	-	-	-	-	-	-	-		
6	46.429	46.433	0.004	0.64	-	-	-	-		
7	48.636	48.621	0.015	0.64	-	-	-	-		
8	50.002	49.993	0.009	0.63	-	-	-	-		
9	50.906	50.892	0.014	0.63	-	-	-	-		
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)
...	-	-	-	-	-	-
∞	54.015	54.015	-	-	-	53.928	53.928	-	-	-

Table 11. Comparison of the present SCUNC calculations of resonance energies (E_n, eV) and quantum defect (δ) of P^{3+} for the following Rydberg serie. $|\Delta E_n|$ denotes the energy difference between the present SCUNC calculations and the experimental data of Hernández et al., 2015 [9].

n	$2p^6 3s^2(^1S_0) \rightarrow 2p^6 3pns\ ^2P_{1/2}$				
	SCUNC E_n	Exp. E_n	$ \Delta E_n $	SCUNC δ	Exp. δ
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
...			
∞	62.435	62.435			

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 $n=30$ 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).

Appendix Detailed Processes to Evaluate Empirically the Screening Constants f_i

In the framework of the Screening constant by unit nuclear (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, Δf_i .

Within the framework of the SCUNC formalism, the screening constants, f_i , are presented as $f_i = f_{i,exp} \pm \Delta f_i$. The

absolute errors, Δf_i are given by Sakho [13].

$$\Delta f_1 = \sqrt{\frac{(f_1 - f_1^+)^2 + (f_1 - f_1^-)^2}{2}} \quad (22)$$

In general, the experimental resonance energies are expressed in the form $E_n = E_{exp} \pm \Delta E$, with ΔE the absolute error on the resonance energies. The f_i^\pm screening constants are evaluated using the experimental resonance energies for $n=v$ for the $nl^{2S+1}L_J$ Rydberg series considered.

As a result, the corrective term in Eq.(5) is equal to zero and we obtain (in Rydberg)

$$E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - \frac{f_1 \left({}^{2s+1}L_J^\pi \right)}{Z(n-1)} - \frac{f_2 \left({}^{2s+1}L_J^\pi \right)}{Z} \right\}^2 \quad (23)$$

In the present work, only f_1 is to be evaluated as $f_2=12.0$ for P^{2+} and $f_2=11.0$ for P^{3+} . In this case, one equation is required to find the value of f_1 in Eq.(23) using the following relations for $n = v$.

$$\begin{cases} E_v^+ = E_{exp} + \Delta E \\ E_v^- = E_{exp} - \Delta E \end{cases} \quad (24)$$

Let us then apply Eq.(24) to evaluate both f_1 and Δf_1 considering for example the Rydberg serie $3s3pnp\ ^3P_0$ originating from the ground state $3s^2 3p(^2P_{1/2})$ of P^{2+} . For these states, the resonance energies are given by Eq.(12) reminded below

$$E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - \frac{f_1(^3P_0, ^2P_{1/2})}{Z(n-1)} - \frac{f_2(^3P_0, ^2P_{1/2})}{Z} - \frac{f_1(^3P_0, ^2P_{1/2})(n-v)}{Z(n+v+2s+7)(n+v-3)} + \frac{f_1(^3P_0, ^2P_{1/2})(n-v)}{Z^2(n+v+s-2)^2} - \frac{f_1(^3P_0, ^2P_{1/2})(n-v)}{Z^3(n+v+s)(n+v+s-1)} \right\}^2$$

For sake of simplification we put $f_1 f_1(^3P_0, ^2P_{1/2})$. The first entry for the Rydberg serie $3s3pnp\ ^3P_0$ originating from the ground state $3s^2 3p(^2P_{1/2})$ is $n = v = 6$. As $Z = 15$ the P^{2+} ion, Eq.(12) above takes the form

$$E_6 = E_\infty - \frac{15^2}{6^2} \left\{ 1 - \frac{f_1}{15(6-1)} - \frac{12}{15} \right\}^2 \times 13.606 = E_\infty - \frac{15^2}{6^2} \left\{ 1 - \frac{f_1}{75} - \frac{12}{15} \right\}^2 \times 13.606 \quad (25)$$

In Table 5 we pull the experimental resonance energy $E_6=(35.451\pm 0.035)eV$, $n=v=6$ from Hernández *et al.*, 2015 [9] along with the energy limits $E_\infty=38.623eV$. Using Eqs.(24) and (25), we find

$$\begin{cases} 35.451 = 38.623 - \frac{15^2}{6^2} \left\{ 1 - \frac{f_1}{75} - \frac{12}{15} \right\}^2 \times 13.606 \\ 35.451 + 0.035 = 38.623 - \frac{15^2}{6^2} \left\{ 1 - \frac{f_1^+}{75} - \frac{12}{15} \right\}^2 \times 13.606 \\ 35.451 - 0.035 = 38.623 - \frac{15^2}{6^2} \left\{ 1 - \frac{f_1^-}{75} - \frac{12}{15} \right\}^2 \times 13.606 \end{cases}$$

Simplifying these equations, we get

$$\begin{cases} 1 - \frac{f_1}{75} - \frac{12}{15} = 0.193135161 \\ 1 - \frac{f_1^+}{75} - \frac{12}{15} = 0.192066674 \\ 1 - \frac{f_1^-}{75} - \frac{12}{15} = 0.194197769 \end{cases} \Rightarrow \begin{cases} f_1 = 0.514862879 \\ f_1^+ = 0.594999398 \\ f_1^- = 0.435167268 \end{cases} \quad (26)$$

Using the results (26) and Eq.(22), the absolute error, Δf_1 is equal to

$$\Delta f_1 = \sqrt{\frac{(0.514862879 - 0.594999398)^2 + (0.514862879 - 0.435167268)^2}{2}} = 0.080$$

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, Δf_i for the remaining series are evaluated similarly.

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