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RESEARCH ARTICLE

SCREENING CONSTANT BY UNIT NUCLEAR CHARGE CALCULATIONS OF THE $3s^23p^4(1D^0)ns$, $3s^23p^4(1D^0)nd$, $3s^23p^4(1S^0)nd$, RYDBERG SERIES FROM METASTABLE STATE OF Ca^{3+} ION

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Abstract

We report in this paper energy positions of the $3s^23p^4(1D^0)ns$, $3s^23p^4(1D^0)nd$, $3s^23p^4(1S^0)nd$, Rydberg series from metastable state of Ca^{3+} ion.. Calculations are performed up to $n = 20$ using the Screening Constant by Unit Nuclear Charge(SCUNC). The present results compared wellwith the experimental data of Ghassan A Alna'washi which are the only available values.The accurate data presented in this work may be a useful guideline for future experimental and other theoretical studies.

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Introduction:-

One of the fundamental processes occurring in astrophysical systems is the photoionization (PI) of atoms and ions according to the single process



Almost all visible matter (less than 5% [1] in the universe is in the plasma form. In hot plasmas, the chemical species (X) of the plasma lose all or part of their electronic procession to find themselves in several states of ionization (X^+ , X^{2+} , X^{3+} , X^{4+} , ...). In addition, a great deal of information about the universe is broadcast by photons [2,3]. Therefore, knowledge of ion-photon interaction processes is essential not only for understanding astrophysical observations but also for modeling laboratory plasmas (thermonuclear fusion by magnetic and inertial confinements). Thus the study of the photoionization of its ions is a crucial interest in astrophysics for the interpretation of astronomical data from stellar systems such as stars and nebulae.

While calcium is not among the most abundant elements in the universe, the amount of calcium predicted by physical models is lower than observed. Also, absorption lines of neutral calcium (CaI) and ionized calcium (CaII) are part of the characteristic spectral lines of many astrophysical systems including stars of class B, A, F, G, K and M . In addition, the discovery of calcium-rich supernovae such as SN 2005E whose calcium nuclei represent nearly half (49%) of the ejected nuclei, i.e. five to ten times more than the number of calcium nuclei found in the two main ones categories of supernova (thermonuclear supernovae (SN Ia) and gravitational supernovae (SN II, SN Ib / Ic) [4].

Thus, the aim of our study is to provide the first theoretical data on the resonance energies of the Ca^{3+} ion.

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In addition, the determination of the photoionization cross section for multicharged atomic systems allows the development of theoretical models of multiple electron interactions [5, 6]. Also, knowledge of the cross section of photoionization leads to accurate values of energies and resonance widths. Thus, many theoretical and experimental methods used in the study of photoionization processes are based on the determination of the cross section of photoionization. However, the complex mathematical formalism of the ab initio methods and the recovery of the peaks of the cross-sections of photoionization from a certain value of the energy of the photons used [2] make it difficult to know the resonance parameters for states of high excitation. Thus, the use of the semi-empirical procedure of the SCUNC method leads to precise results for the energies and resonance widths of the Rydberg series without making use of a complex mathematical formalism.

The Screening Constant by Unit Nuclear Charge (SCUNC) formalism presented by Sakho[7][8][9] is seen to be a very suitable semi-empirical photoionization method for reproducing excellently high experimental data. The goal of the present study is to enlighten the superimposed ALS lines using the SCUNC method for calculating resonances energies of the $3s^23p^4(^1D^o)ns$, $3s^23p^4(^1D^o)nd$, $3s^23p^4(^1S^0)nd$, Rydberg series of Ca^{3+} ion. The only studies on this atomic system have been made, at the Advanced Light Source (ALS) located in the United States, by Ghassan A. Alna'washi and his group using the technique of collinear beams (merge an ion beam with a photon beam). In this work, we aim to extend the ALS experiments of Ghassan A. Alna'washi[2] along with their DARC calculations to the high lying. Analysis of the present results is achieved in the framework of the standard quantum-defect theory and of the SCUNC-procedure by calculating the effective charge. The present paper is organized as follows. Section 2 presents a brief outline of the theoretical part of the work. In section 3, we present and discuss our results compared with the available experimental results. In section 4, we summarize our study and draw conclusions.

Theory

Brief description of the SCUNC formalism

In the framework of the Screening Constant by Unit Nuclear Charge formalism, the total energy of the $(Nl, nl')^{2S+1}L^\pi$ excited states is expressed in the form (in Rydberg)

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

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 [9]

$$\beta(Nl, nl'; 2S+1L^\pi; Z) = \sum_{k=1}^q f_k \left(\frac{1}{Z} \right)^k. \quad (3)$$

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

For a given Rydberg series originating from a $^{2S+1}L_J$ state, we obtain using [9]

$$E_n = E_\infty - \frac{Z^2}{n^2} \left[1 - \beta(nl; s, \mu, \nu, 2S+1L^\pi; Z) \right]^2 \quad (4)$$

In this equation, ν and μ ($\mu > \nu$) denote the principal 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 ($s = 1/2$), I_k is the K-shell ionization energy, 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

$$\beta(Z, {}^{2S+1}L_J, n, s, \mu, \nu) = \sum_{k=1}^q f_k \left(\frac{1}{Z}\right)^k. \quad (5)$$

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[9]

$$E_n = E_\infty - \frac{Z^2}{n^2} \left\{ 1 - \frac{f_1({}^{2S+1}L^\pi)}{Z(n-1)} - \frac{f_2({}^{2S+1}L^\pi)}{Z} \pm \sum_{k=1}^q \sum_{k'=1}^{q'} f_1^{k'} F(n, \mu, \nu, s) \times \left(\frac{1}{Z}\right)^k \right\}^2 \quad (6)$$

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 introduce to stabilize the resonance energies

with increasing the principal quantum number n . In general, resonance energies are analyzed from the standard quantum-defect expansion formula

$$E_n = E_\infty - \frac{RZ_{core}^2}{(n-\delta)^2}. \quad (7)$$

In this equation, R is the Rydberg constant, E_∞ the energy limit of the series, Z_{core} represents the electric charge of the 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 [9]

$$E_n = E_\infty - \frac{Z^{*2}}{n^2} R. \quad (8)$$

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

$$Z^* = \frac{Z_{core}}{\left(1 - \frac{\delta}{n}\right)}. \quad (9)$$

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

$$\begin{cases} Z^* \geq Z_{core} & \text{if } \delta \geq 0 \\ Z^* \leq Z_{core} & \text{if } \delta \leq 0. \end{cases} \quad (10)$$

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

Besides, comparing Eq. (6) and Eq. (8), the effective charge is in the form

$$Z^* = Z \left\{ 1 - \frac{f_1({}^{2S+1}L^\pi)}{Z(n-1)} - \frac{f_2({}^{2S+1}L^\pi)}{Z} \pm \sum_{k=1}^q \sum_{k'=1}^{q'} f_1^{k'} F(n, \mu, \nu, s) \times \left(\frac{1}{Z}\right)^k \right\}. \quad (11)$$

Besides, the f_2 -parameter in Eq. (3) can be theoretically determined from Eq. (11)

$$\lim_{n \rightarrow \infty} Z^* = Z \left(1 - \frac{f_1 \left(\frac{2S+1}{Z} L^\pi \right)}{Z} \right) = Z_{core} \quad (12)$$

We get then $f_2 = Z - Z_{core}$, where Z_{core} is directly obtain by the photoionization process from an atomic X^{p+} system $X^{p+} + h\nu \rightarrow X^{(p+1)+} + e^-$. We find then $Z_{core} = p + 1$. So, for the Ca^{3+} ions, $Z_{core} = 4$. The remaining f_1 -parameter is to be evaluated empirically using the experimental data from Advanced Light Source (ALS) experiments of Ghassan A. Alna'washi[2] for a given $(^{2S+1}L_J) \mu l$ level.

Energy resonances of the Rydberg series from metastable state of Ca^{3+} ion.

Using Eq. (6), we obtain the following energy positions (in Rydberg)

- For the $3s^2 3p^5 \ ^2P_{1/2}^o \rightarrow 3s^2 3p^4 (\ ^1D) nd (\ ^2D)$ transitions :

$$E_n = E_\infty - \frac{Z^2}{n^2} \left[1 - \frac{f_1}{Z(n-1)} - \frac{f_2}{Z} - \frac{f_1}{Z^2} \times \frac{(n-\mu)(n-\nu)}{(n-\mu+s)^2 (n-\nu+s)^2} - \frac{f_1}{Z^3} \times \frac{(n-\mu)(n-\nu)}{(n-\mu+s)(n-\nu-s)} \right]^2 \quad (13)$$

The screening constants in (13) are determined from the transition energy measured by Ghassan A. Alna'washi[2]. Using the experimental data of ALS Ghassan A. Alna'washi[2], we obtain (in eV) $E_\nu = E_{10} = 66.758 \pm 0.015$ ($\nu = 10$) and $E_\mu = E_{11} = 67.314 \pm 0.015$ ($\mu = 11$) respectively for the $3s^2 3p^5 \ ^2P_{1/2}^o \rightarrow 3s^2 3p^4 (\ ^1D) 10d (\ ^2D)$ and $3s^2 3p^5 \ ^2P_{1/2}^o \rightarrow 3s^2 3p^4 (\ ^1D) 11d (\ ^2D)$ transitions. From NIST [10], we find $E_\infty = 69.398$ eV. Using these data, Eq. (13) gives $f_1 = -8.98903563 \pm 0.26814235$; $f_2 = 16.5937616 \pm 0.04230792$

- For the $3s^2 3p^5 \ ^2P_{1/2}^o \rightarrow 3s^2 3p^4 (\ ^1D) nd (\ ^2P)$ transitions :

$$E_n = E_\infty - \frac{Z^2}{n^2} \left[1 - \frac{f_1}{Z(n-1)} - \frac{f_2}{Z} - \frac{f_1}{Z^2} \times \frac{(n-\mu)(n-\nu)}{(n-\mu+s)^2 (n-\nu+s)^2} \right]^2 \quad (14)$$

For the $3s^2 3p^5 \ ^2P_{1/2}^o \rightarrow 3s^2 3p^4 (\ ^1D) 10d (\ ^2P)$ and $3s^2 3p^5 \ ^2P_{1/2}^o \rightarrow 3s^2 3p^4 (\ ^1D) 11d (\ ^2P)$ transitions, we find using the experimental data of ALS Ghassan A. Alna'washi[2], $E_\nu = E_{10} = 66.733 \pm 0.015$ ($\nu = 10$) and $E_\mu = E_{11} = 67.289 \pm 0.015$ ($\mu = 11$). From NIST [10], we find $E_\infty = 69.398$ eV. Eq. (14) provides then $f_1 = -8.54464722 \pm 0.2651479$ and $f_2 = 16.5235771 \pm 0.04191635$

- For the $3s^2 3p^5 \ ^2P_{1/2}^o \rightarrow 3s^2 3p^4 (\ ^1D) nd (\ ^2S)$ transitions:

$$E_n = E_\infty - \frac{Z^2}{n^2} \left[1 - \frac{f_1}{Z(n-1)} - \frac{f_2}{Z} - \frac{f_1}{Z^2} \times \frac{(n-\mu)(n-\nu)}{(n-\mu+3s)(n-\nu+s)} \right]^2 \quad (15)$$

For the $3s^2 3p^5 \ ^2P_{1/2}^o \rightarrow 3s^2 3p^4 (\ ^1D) 10d (\ ^2S)$ and $3s^2 3p^5 \ ^2P_{1/2}^o \rightarrow 3s^2 3p^4 (\ ^1D) 11d (\ ^2S)$ transitions, the experimental energy positions ALS Ghassan A. Alna'washi[2], are $E_\nu = E_{10} = 66.993 \pm 0.015$ ($\nu = 10$) and $E_\mu = E_{11} = 67.424 \pm 0.015$ ($\mu = 11$). From NIST [10], we find $E_\infty = 69.398$ eV. In that case, we find using Eq. (15) $f_1 = -1.29710682 \pm 0.25272327$ and $f_2 = 15.9397283 \pm 0.04119184$

- For the $3s^2 3p^5 \ ^2P_{1/2}^o \rightarrow 3s^2 3p^4 (\ ^1D) ns (\ ^2D_{3/2})$ transitions:

$$E_n = E_\infty - \frac{Z^2}{n^2} \left[1 - \frac{f_1}{Z(n-1)} - \frac{f_2}{Z} + \frac{f_1}{Z^2} \times \frac{(n-\mu)(n-\nu)}{(n-\mu+s)^2(n-\nu+s)} \right]^2 \quad (16)$$

From ALS of Ghassan A. Alna'washi[2], we obtain for the $3s^23p^5\ ^2P_{1/2} \rightarrow 3s^23p^4(^1D)11s(^2D_{3/2})$ and $3s^23p^5\ ^2P_{1/2} \rightarrow 3s^23p^4(^1D)12s(^2D_{3/2})$ $E_\nu = E_{11} = 67.384 \pm 0.015$ ($\nu = 11$) and $E_\mu = E_{12} = 67.724 \pm 0.015$ ($\mu = 12$). From NIST [10], we find $E_\infty = 69.398$ eV. We find then using Eq. (16) $f_1 = -2.5266269 \pm 0.34080818$ and $f_2 = 16.0204415 \pm 0.04984143$.

• For the $3s^23p^5\ ^2P_{1/2}^o \rightarrow 3s^23p^4(^1S)nd(^2D)$ transitions:

$$E_n = E_\infty - \frac{Z^2}{n^2} \left[1 - \frac{f_1}{Z(n-1)} - \frac{f_2}{Z} + \frac{f_1}{Z^2} \times \frac{(n-\mu)(n-\nu)}{(n-\mu+s)^2(n-\nu+s)^2} + \frac{f_1}{Z^3} \times \frac{(n-\mu)(n-\nu)}{(n-\mu+s)^2(n-\nu+3s)} \right]^2 \quad (17)$$

From ALS of Ghassan A. Alna'washi[2], we obtain for $3s^23p^5\ ^2P_{1/2} \rightarrow 3s^23p^4(^1S)7d(^2D)$ and $3s^23p^5\ ^2P_{1/2} \rightarrow 3s^23p^4(^1S)8d(^2D)$ $E_\nu = E_7 = 67.691 \pm 0.015$ ($\nu = 7$) and $E_\mu = E_8 = 68.882 \pm 0.015$ ($\mu = 8$). From NIST [10], we find $E_\infty = 72.498$ eV. We find then using Eq. (17) $f_1 = -1.53473413 \pm 0.08662243$ and $f_2 = 16.0949488 \pm 0.02092893$

• For the $3s^23p^5\ ^2P_{1/2}^o \rightarrow 3s^23p^4(^1S)nd(^2S_{1/2})$ transitions:

$$E_n = E_\infty - \frac{Z^2}{n^2} \left[1 - \frac{f_1}{Z(n-1)} - \frac{f_2}{Z} - \frac{f_1}{Z^2} \times \frac{(n-\mu)(n-\nu)}{(n-\mu+s)(n-\nu-s)} - \frac{f_1}{Z^3} \times \frac{(n-\mu)(n-\nu)}{(n-\mu+s)(n-\nu+2s)} \right]^2 \quad (18)$$

From ALS of Ghassan A. Alna'washi[2], we obtain for the $3s^23p^5\ ^2P_{1/2} \rightarrow 3s^23p^4(^1S)7d(^2S_{1/2})$ and $3s^23p^5\ ^2P_{1/2} \rightarrow 3s^23p^4(^1S)8d(^2S_{1/2})$ $E_\nu = E_7 = 67.880 \pm 0.015$ ($\nu = 7$) and $E_\mu = E_8 = 69.050 \pm 0.015$ ($\mu = 8$). From NIST [10], we find $E_\infty = 72.498$ eV. We find then using Eq. (18) $f_1 = -2.16111559 \pm 0.08980098$ and $f_2 = 16.2819632 \pm 0.021590$.

Results and Discussion:-

The results of our calculations on the resonance energies (in eV) of the Rydberg series of the Ca^{3+} ion are listed in Tables 1-6. They are compared with the experimental ALS (Advanced Light Source) values of Ghassan A. Alna'washi et al (2010)[2] which are to our knowledge the only values available on the resonance energies of the Rydberg series for the Ca^{3+} ion. Overall our results are in perfect agreement with these experimental values. They also meet the SCUNC analysis conditions which become:

$$\begin{cases} Z^* \geq 4 & \text{if } \delta \geq 0 \\ Z^* \leq 4 & \text{if } \delta \leq 0 \\ \lim_{n \rightarrow \infty} Z^* = 4 \end{cases}$$

Table 1 shows the SCUNC resonances energy of the $3s^23p^4(^1D)nd(^2D)$ Rydberg series originating from the metastable state of the Ca^{3+} ion. For this Rydberg series we calculated the energies of the first eleven self-ionizing states. The effective charges of these resonant states satisfy the conditions for SCUNC analysis. Regarding the quantum defect, the difference between two consecutive levels is 0.15 except for the second and third resonant states. It is seen that the energy differences are less than 0.010 eV. This may expect our results up to $n = 20$ to be accurate.

Table 2 lists the SCUNC energies of the first eleven auto-ionizing states of the $3s^23p^4(^1D)nd(^2P)$ Rydberg series originating from the metastable state of the Ca^{3+} ion. The quantum defect of these resonant states decreases on average by 0.15 when the principal quantum number increases. For $n = 17$ up to $n = 20$, Quantum defects are

negative because the effective charges of these self-ionizing states are less than the charge of the Ca^{4+} ion, and if not, they are positive. The agreements between the SCUNC results and experimental data are seen to be very good. This allows us to expect our results on the resonance energies for this Rydberg series up to $n=20$ to be accurate.

In Tables 3, we show a comparison of the energy resonances (SCUNC) and quantum defect (δ) of the $3s^2 3p^4 ({}^1D) nd ({}^2S)$ Rydberg series originating from the metastable state of the Ca^{3+} ion. The effective charges of the first eleven resonant states of this Rydberg series are all greater than the charge of the Ca^{4+} ion because all quantum defects are positive and verify the SCUNC analysis conditions. We note that quantum defect increases so lightly and monotonously which agrees well with the analysis condition. Our results on the resonance energies of this Rydberg series can therefore be considered to be accurate.

In Table 4, we list the present energy resonances (SCUNC) and quantum defect (δ) for the first ten resonant states of the $3s^2 3p^4 ({}^1D) ns ({}^2D_{3/2})$ Rydberg series originating from the metastable state of the Ca^{3+} ion. For this series, except for the first two auto-ionizing states which have a quantum defect equal to 0.6, the other resonant states have a quantum defect that is equal to 0.5 or near to this value. Moreover, along the series, the quantum defects are positive because the effective charges of the resonant states are greater than the charge of the Ca^{4+} ion. Here again, the agreements are seen to be very good. For both experiment and theory, the energy differences have never overrun 0.001 eV. This justifies to expect our results for the resonance energies of this series up to $n = 20$ to be accurate.

In Table 5, we compare the present (SCUNC) energy resonances and quantum defect (δ) of the $3s^2 3p^4 ({}^1S) nd ({}^2D)$ Rydberg series originating from the metastable state of the Ca^{3+} ion. For this Rydberg series, the quantum defect decreases when the principal quantum number increases. The maximum decrease is equal to 0.04 and takes place between the second and third resonant states. Also the effective charges of the fourteen resonant states for which we calculated the energies are in agreement with the conditions of SCUNC analysis. This allows us to expect our results to be accurate up to $n = 20$.

In Table 6, we quote the present SCUNC results for energy resonances and quantum defect (δ) of the first fourteen auto-ionizing states of the Rydberg series originating from the metastable state of the Ca^{3+} ion. For the first three levels of this series, the quantum defect behaves in the same way as that obtained from the ALS experiment. The quantum defect of the other resonant states decreases when the principal quantum number increases. The effective charges of this series are greater than the charge of the Ca^{4+} ion only for the first four levels while the quantum defects of the other levels are negative. This may expect our results for $n > 9$ to be accurate.

For all the Rydberg series investigated, the slight discrepancies between the present calculations and experiment may be explained by the simplicity of the SCUNC formalism which does not include explicitly any relativistic corrections.

Conclusions:-

The Screening Constant by Unit Nuclear Charge (SCUNC) formalism has been applied to the photoionization of the $3s^2 3p^4 ({}^1D^o) ns$, $3s^2 3p^4 ({}^1D^o) nd$, $3s^2 3p^4 ({}^1S^o) nd$, Rydberg series of Ca^{3+} ion. Overall, the results obtained compared very well with available literature data. New high lying accurate resonance energies are tabulated as benchmarked data. Over the entire Rydberg series investigated, it is shown that the present SCUNC results agree very well with the only available experimental data of ALS of Ghassan A. Alna'washi et al (2010)[2]. A host of accurate data up to $n = 20$ are quoted in the recent work. The very good results obtained in this work point out the possibilities to use the SCUNC formalism in the investigation of high lying Rydberg series of ions containing several electrons in the framework of a soft procedure. This work may be of interest for future experimental and theoretical studies in the photoabsorption spectrum of Ca^{3+} .

Credit author statement

Malick SOW: Conceptualization; Methodology, Software, Formal analysis, validation, Data curation, Writing-Original draft preparation; Writing- Reviewing and Editing, Validation.

Papa Amadou Lamine Diagne: Software; Formal analysis, Validation.

Fatou Ndoye: Software; Formal analysis, Validation.

Momar Talla Gning: Software; Formal analysis, Validation.

Babou DIOP:Software, Visualization, Formal analysis, Validation.

IbrahimaSakho: Conceptualization; Methodology,Software, Visualization, Formal analysis, Validation

Table 1:- Resonance energies E_n , quantum defects (Ξ) and effective charges (Z^*) of the $3s^2 3p^4(^1D)nd(^2D)$ Rydberg series from the metastable state of the Ca^{3+} ion. The present results (SCUNC) are expressed in eV and compared to the Advanced Light Source (ALS) data of Ghassan A. Alna'washi et al (2010)[2].

n	E_n		Ξ	δ		Z^*
	SCUNC	ALS		SCUNC	ALS	
10	66.758	66.758	0.000	0.92	0.92	4.405
11	67.314	67.314	0.000	0.78	0.78	4.305
12	67.672	67.674	0.008	0.77	0.76	4.274
13	67.983	—	—	0.60	—	4.192
14	68.215	—	—	0.44	—	4.128
15	68.393	—	—	0.28	—	4.076
16	68.534	—	—	0.13	—	4.032
17	68.647	—	—	-0.03	—	4.025
18	68.739	—	—	-0.18	—	4.020
19	68.815	—	—	-0.33	—	4.018
20	68.879	—	—	-0.48	—	4.017
⋮						
∞^a 69.398						

^aNIST atomic database [10].

Ξ : energy differences relative to the experimental data

Table 2:- Resonance energies E_n , quantum defects (Ξ) and effective charges (Z^*) of the $3s^2 3p^4(^1D)nd(^2P)$ Rydberg series from the metastable state of the Ca^{3+} ion. The present results (SCUNC) are expressed in eV and compared to the Advanced Light Source (ALS) data of Ghassan A. Alna'washi et al (2010) [2].

n	E_n		Ξ	δ		Z^*
	SCUNC	ALS		SCUNC	ALS	
10	66.733	66.733	0.000	0.96	0.96	4.426
11	67.289	67.289	0.000	0.84	0.84	4.331
12	67.661	67.659	0.002	0.81	0.81	4.290
13	67.971	—	—	0.65	—	4.210
14	68.204	—	—	0.50	—	4.148
15	68.383	—	—	0.36	—	4.097
16	68.525	—	—	0.21	—	4.054
17	68.638	—	—	0.07	—	4.017
18	68.731	—	—	-0.07	—	4.010
19	68.808	—	—	-0.21	—	4.008
20	68.873	—	—	-0.36	—	4.007
⋮						
∞^a 69.398						

^aNIST atomic database [10].

Ξ : energy differences relative to the experimental data

Table 3:- Resonance energies E_n , quantum defects (Ξ) and effective charges (Z^*) of the $3s^2 3p^4(^1D)nd(^2S)$ Rydberg series from the metastable state of the Ca^{3+} ion. The present results (SCUNC) are expressed in eV and compared to the Advanced Light Source (ALS) data of Ghassan A. Alna'washi et al (2010) [2].

n	E_n		Ξ	δ		Z^*
	SCUNC	ALS		SCUNC	ALS	
10	66.993	66.993	0.000	0.49	0.49	4.204
11	67.424	67.424	0.000	0.50	0.50	4.190
12	67.742	67.739	0.003	0.55	0.55	4.191

13	67.985	—	—		0.59	—	4.189
14	68.181	—	—		0.63	—	4.187
15	68.339	—	—		0.66	—	4.185
16	68.468	—	—		0.70	—	4.184
17	68.574	—	—		0.74	—	4.183
18	68.664	—	—		0.78	—	4.182
19	68.739	—	—		0.82	—	4.182
20	68.803	—	—		0.87	—	4.182
⋮							
∞ ^a	69.398						

^aNISTatomicdatabase [10].

Ξ: energydifferences relative to the experimental data

Table 4:- Resonance energies E_n , quantum defects (δ) and effective charges (Z^*) of the $3s^2 3p^4 ({}^1D) ns ({}^2D_{3/2})$ Rydberg series from the metastable state of the Ca^{3+} ion. The present results (SCUNC) are expressed in eV and compared to the Advanced Light Source (ALS) data of Ghassan A. Alna'washi et al (2010) [2].

n	E_n		Ξ		δ		Z^*
	SCUNC	ALS			SCUNC	ALS	
11	67.384	67.384	0.000		0.60	0.60	4.232
12	67.724	67.724	0.000		0.60	0.60	4.209
13	68.005	68.004	0.001		0.50	0.50	4.161
14	68.203	—	—		0.51	—	4.150
15	68.362	—	—		0.51	—	4.139
16	68.492	—	—		0.50	—	4.130
17	68.598	—	—		0.50	—	4.121
18	68.688	—	—		0.50	—	4.113
19	68.763	—	—		0.49	—	4.106
20	68.826	—	—		0.48	—	4.099
⋮							
∞ ^a	69.398						

^aNISTatomicdatabase [10].

Ξ: energydifferences relative to the experimental data

Table 5:- Resonance energies E_n , quantum defects (δ) and effective charges (Z^*) of the $3s^2 3p^4 ({}^1S) nd ({}^2D)$ Rydberg series from the metastable state of the Ca^{3+} ion. The present results (SCUNC) are expressed in eV and compared to the Advanced Light Source (ALS) data of Ghassan A. Alna'washi et al (2010)[2].

n	E_n		Ξ		δ		Z^*
	SCUNC	ALS			SCUNC	ALS	
7	67.691	67.691	0.000		0.27	0.27	4.161
8	68.882	68.882	0.000		0.24	0.24	4.124
9	69.688	69.686	0.002		0.20	0.20	4.092
10	70.242	—	—		0.18	—	4.072
11	70.648	—	—		0.15	—	4.056
12	70.954	—	—		0.13	—	4.043
13	71.190	—	—		0.10	—	4.031
14	71.375	—	—		0.08	—	4.022
15	71.524	—	—		0.05	—	4.014
16	71.645	—	—		0.03	—	4.006
17	71.745	—	—		0.01	—	4.005
18	71.828	—	—		-0.02	—	4.003
19	71.898	—	—		-0.05	—	4.002
20	71.958	—	—		-0.07	—	4.001

n	E_n		Ξ	δ		Z^*
	SCUNC	ALS		SCUNC	ALS	
7	67.880	67.880	0.000	0.13	0.13	4.078
8	69.051	69.051	0.000	0.04	0.05	4.027
9	69.767	69.766	0.001	0.06	0.07	4.033
10	70.307	—	—	0.01	—	4.013
11	70.702	—	—	-0.03	—	4.011
12	70.998	—	—	-0.08	—	4.010
13	71.226	—	—	-0.12	—	4.009
14	71.405	—	—	-0.17	—	4.008
15	71.548	—	—	-0.20	—	4.007
16	71.665	—	—	-0.24	—	4.006
17	71.761	—	—	-0.28	—	4.005
18	71.841	—	—	-0.31	—	4.004
19	71.908	—	—	-0.34	—	4.003
20	71.965	—	—	-0.37	—	4.002

^aNISTatomicdatabase [10].

Ξ : energydifferences relative to the experimental data.

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Conflicts of Interest:

The authorsdeclare no conflicts of interestregarding the publication of this paper.

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