

RESEARCH ARTICLE

PHOTOIONIZATION STUDY OF THE SINGLETS [1S²2P(²P_{3/2})NS ¹P, 1S²2P (²P)ND ¹P, 1S²2P (²P_{1/2})NP ¹P, $1S^{2}2P (^{2}P_{3/2})NP ^{1}D]$ AND TRIPLETS $[1S^{2}2P (^{2}P^{0})NS ^{3}P_{0,1,2}]$ RYDBERG SERIES FOR THE NIV IONS VIA THE MODIFIED ATOMIC ORBITAL THEORY

Abdou Faye, Malick Sow, Moustapha Kebe, Ndeye Astou Thiam, Sory Diaw, Omar Baba Dia, Papa Mamadou Ndiaye and Cheikh Tidiane Diouf

Department of Physics, Faculty of Sciences and Technologies, University Cheikh Anta DIOP of Dakar, Dakar, Senegal.

Abstract

Manuscript Info

Manuscript History Received: 24 August 2024 Final Accepted: 28 September 2024 Published: October 2024

Key words:-Rydberg Photoionization, Series. Doubley-Excuted States, MAOT, Ouantum Defect, Atoms and Ions

..... In this paper, we report resonance energies and quantum defect of the singlets 1s²2p (²P_{3/2})ns ¹P, 1s²2p (²P)nd ¹P, 1s²2p (²P_{1/2})np ¹P, 1s²2p $({}^{2}P_{3/2})$ np ${}^{1}D$ and triplets $1s^{2}2p$ (${}^{2}P^{o}$)ns ${}^{3}P_{0,1,2}$, Rydberg series from the ground state of N^{3+} (NIV) ions. Calculations are performed from n =3 to n = 20 using the Modified Atomic Orbital Theory (MOAT) Very good agreements are seen between the present formalism. calculations and the available theoretical and experimental data. The present predicted data up to n = 20 may be a great importance for the atomic physics communityin connection with the understanding of the chemical evolution of the N element in the Universe.

Copyright, IJAR, 2024,. All rights reserved.

Introduction:-

The study of the photoionization of atoms and ions is a fundamental process which is very important in many fields of astrophysics, notably stars, astrophysical plasmas, fusion with inertial confinement. The photoionization of ions counteracts plasma opacity and radiation transfer in plasmas [1] [2].

The photoionization of Be-like ions allows to study the electronic correlation of the simple multishell atomic systems, a large number of studies such as PI cross sections, energies and widths of the doubly excited states and oscillating forces for beryllium. The isoelectronic sequences have been carried out in recent decades. The isoelectronic sequences of type Be appear to be a slightly more complicated system than helium and helium ions. Thus, intensive research has been carried out both at the experimental and theoretical level to study the processes of photoionization resonance of the atom of the Be type. Many studies on resonance parameters (PI cross sections, energies and widths) of doubly excited states and oscillating forces for beryllium as well as isoelectronic sequences have been carried out in the last decades. By way of illustration, Berrington et al. [3] had studied the PI cross-section of the isoelectronic sequence Be using R-matix and thus obtained an approximate figure of the PI cross-section for N IV. In addition, Garcia et al. [4] studied high energy photoabsorption sections for nitrogen ions in the region of the K edge, and obtained the energies of the K-level vacuum, the wavelengths, Einstein's coefficients, radiative widths and Auger's N IV based on the R matrix method of Breit-Pauli.

Using the MAOT method [5:6], Sow et al. [7] reported accurate energy positions for the singlets and triplets 2pns 1,3 PO and 2pnd 1,3 P⁰ levels of the Beryllium atom up to n = 25 along with resonance width. In this paper, these previous study are extended to the photoionization of the Be- like N3+ ions in the framework of MAOT formalism. The MAOT method is known to be a very suitable technique of calculation that has given recently accurate results from simple semi-empirical formulas without needing to compute any photoionization cross section. Recently, Sow et al. [6][7] [8] demonstrated the possibility of the Modified Atomic Orbital Theory to reproduce experimental data with great precision. The purpose of the present work is to report accurate results for energy positios of the singlets $[1s^22p (^2P_{3/2})ns \ ^1P, 1s^22p (^2P_{3/2})nd \ ^1P, 1s^22p (^2P_{1/2})np \ ^1P, 1s^22p (^2P_{1/2})np \ ^1D]$, and triplets $[1s^22p (^2P^o)ns \ ^3P_0, 1s^22p (^2P^o)ns \ ^3P_1$ and $1s^22p (^2P^o)ns \ ^3P_2$] Rydberg series of Be-like nitrogen (N³⁺ ions) from ground state. The analysis of the results is carried out by the MAOT procedure with the quantum defect theory δ .

Section 2 presents the theoretical procedure adopted in this work with a brief description of the MAOT formalism and the analytical expressions used in the calculations. In Section 3, we present and discuss the results obtained along with comparison with the only available R-Matrix theoretical calculatins of Liang et al.[9] and experimental data of Kramidal et al. [10]. In Section 4, we will summarize our study and draw conclusions.

Theory

Brief Description of the MOAT formalism

In the framework of the Modified Atomic Orbital Theory (MAOT), total energy of a (vl)- given orbital is expressed in the form [5] [6] [7].

$$E = -\frac{\left[Z - \sigma(\ell)\right]^2}{\nu^2}$$

For an atomic system of several electrons M, the total energy is given by (in Rydberg) :

$$E = -\sum_{i=1}^{M} \frac{[Z - \sigma_i(\ell)]^2}{v_i^2}$$
(2)

With respect to the usual spectroscopic notation $(N\ell, n\ell)^{2S+1}L^{\pi}$, this equation becomes

$$E = -\sum_{i=1}^{M} \frac{[Z - \sigma_i (2^{S+1} L^{\pi})]^2}{V_i^2}.$$
(3)

(1)

In the photoionization of atoms and ions, energy resonances are generally measured relatively to the E_{∞} converging limit of a given $({}^{2S+1}L_J)nl - Rydberg$ serie. For these states, the general expression of the energy resonance E_n is given

$$E_{n} = E_{\infty} - \frac{1}{n^{2}} \left\{ Z - \sigma_{1} (^{2S+1}L_{J}) - \sigma_{2} (^{2S+1}L_{J}) \times \frac{1}{n} - \sigma_{2}^{\alpha} (^{2S+1}L_{J}) \times (n-m) \times (n-q) \sum_{k} \frac{1}{f_{k}(n,m,q,s)} \right\}^{2}$$
(4)

In this equation, m and q (m < q) denote the principal quantum numbers of the $\sigma i ({}^{2s+1}L_J)nl - Rydberg$ serie of the considered atomic system used in the empirical determination of the $\sigma i ({}^{2s+1}L_J)$ -screening constants s represents

considered atomic system used in the empirical determination of the C_{J} -screening constants s represents the spin of the nl-electron (s= $\frac{1}{2}$), E_{∞} is the energy value of the serie limit generally determined from National Institute of Standards and Technology (NIST) atomic database E_n , denote correspondaient energy resonance and Z represents the nuclear charge of the considered element. The only problem that one lay face by using the MAOT

$$\sum_{k} \frac{1}{f_k(n,m,q,s)}$$

formalism is linked to the determination of the $\overline{k} f_k(n, m, q, s)$ -term. The correct expression of this ter mis determined iteratively by imposing general Eq. (4) to give accurate data with a constant quantum defect values along all the considered series. The value of α is generally fixed to 1 and or 2 during the iteration. The standard quantum defect expansion is given as follows :

$$E_n = E_{\infty} - \frac{RZ_{core}^2}{\left(n - \delta\right)^2} \tag{5}$$

In the equation, R, E_{∞} , Z_{core} and δ are the Rydberg constant, the converging limit, the electric charge of the core ion and the quantum defect, respectively.

 Z_{core} is directly obtained by the photoionization process from an atomic X^{p+} system :

$$X^{p+} + h\nu \rightarrow X^{(p+1)+} + e^{-}.$$
 We find then $Z_{\text{core}} = p+1.$ (6)
From equation (6) we obtain the expression for the quantum defect.

From equation (6) we obtain the expression for the quantum defect δ :

$$\delta = n - Z_{core} \times \sqrt{\frac{R}{(E_{\infty} - E_n)}}$$
⁽⁷⁾

Resonances Energy of the singlets $1s^22p$ (²P_{3/2})ns ¹P, $1s^22p$ (²P)nd ¹P, $1s^22p$ (²P_{1/2})np ¹P, $1s^22p$ (²P_{1/2})np ¹D and the triplets $1s^22p$ (²P⁰)ns ³P_{0,1,2} Rydberg Series of the N³⁺ ions.

In the framework of the MAOT formalism the energy positions of the singlet $1s^22p(^2P)ns^{-1}P$, $1s^22p(^2P)nd^{-1}P$, $1s^22p(^2P_{1/2})np^{-1}P$, $1s^22p(^2P_{1/2})np^{-1}D$ and triplet $1s^22p(^2P^o)ns^{--3}P_{0,1,2}$ Rydberg Series are given (in Rydberg units) by using the general Eq.(4). Thus :

For the $1s^2 2p ({}^2P^0_{3/2})ns {}^1P$ levels

$$E_{n} = E_{\infty} - \frac{1}{n^{2}} \left\{ Z - \sigma_{1} - \frac{\sigma_{2}}{n} - \sigma_{2} \times (n - m) \times (n - q) \times \left[\frac{1}{(n + s)^{2} (n + m + q - s)^{2}} + \frac{1}{(n - m + q + 6s)^{4}} + \frac{1}{(n + 2m - q + 9s)^{5}} \right] \right\}^{2}$$
(8)

To evaluate the σ_i -screening constants (i =1,2), we use the experimental data Eexp [2p(²P_{3/2})nl ¹P] of Kramidal et al.[10].

Thus, for the 1s²2p (${}^{2}P_{3/2}$)3s ${}^{1}P$ and 1s²2p (${}^{2}P_{3/2}$)4s ${}^{1}P$ levels, we respectively get (in Rydberg units) $E_m = E_3 = 4.3105560 \text{ (m = 3)}$ and $E_q = E_4 = 5.292799 \text{ (q = 4)}$. From NIST, we find $E_{\infty} = 6.429778$ Ry. Using these data, eq. (8) gives : $\sigma_1 = 3.041106$ and $\sigma_2 = -1.225098$.

For the $1s^2 2p ({}^2P^{0}_{3/2})nd^{-1}P$ levels

$$E_{n} = E_{\infty} - \frac{1}{n^{2}} \left\{ Z - \sigma_{1} - \frac{\sigma_{2}}{n} - \sigma_{2} \times (n - m) \times (n - q) \times \left[\frac{1}{(n - m + q + 2s) \times (n + 5s)^{3}} + \frac{1}{(n - 2m + q + 8s)^{4}} \right] \right\}^{2}$$
(9)

Using the exprimental data of Kramidal et al.[10]., we obtain in Ryberg $E_m = E_5 = 5.79991$ (m=5) and $E_q = E_6 = 5.99060$ (q=6) of the 1s²2p (²P_{3/2})5d ¹P and 1s²2p (²P_{3/2})4s ¹P respectively. From NIST data, we find $E_{\infty} = 6.429778$ Ry. This data allows us to obtain, using the equation (9) : $\sigma_1 = 2.983674$ and $\sigma_2 = 0.240576$.

For the $1s^2 2p ({}^2P^{0}_{1/2})np {}^1P$ levels

$$E_{n} = E_{\infty} - \frac{1}{n^{2}} \left\{ Z - \sigma_{1} - \frac{\sigma_{2}}{n} - \sigma_{2} \times (n - m) \times (n - q) \times \left[\frac{1}{(n - m + q + 2s)^{3}} + \frac{1}{(n - m + 2q + 7s)^{4}} \right] \right\}^{2}$$
(10)

From the exprimental data of Kramidal et al.[10], we obtain for the $1s^22p ({}^2P_{1/2})3p {}^1P$ and $1s^22p ({}^2P_{1/2})4p {}^1P$, $E_m = E_3 = 4.55365 \text{ (m=3)}$ and $E_q = E_4 = 5.386143 \text{ (q=4)}$. From NIST, we find $E_{\infty} = 6.427421 \text{ Ry}$. We find then using eq. (10), we obtain $\sigma 1 = 3.092583$ and $\sigma 2 = -1.148161$.

For the 1s^2 2p ({}^2P^{o}_{3/2})np {}^1D levels

$$E_{n} = E_{\infty} - \frac{1}{n^{2}} \left\{ Z - \sigma_{1} - \frac{\sigma_{2}}{n} - \sigma_{2} \times (n - m) \times (n - q) \times \left[\frac{1}{(n + s + 1)^{2} \times (n - m + q + 4s)^{3}} \right] \right\}$$

$$+\frac{1}{(n+m+q+5s)^4} + \frac{1}{(n-m+q+9s)^5} + \frac{1}{(n+m+q+9s)^6} \right]^2$$
(11)

For the 1s²2p ($^{2}P_{3/2}^{\circ}$)3p ^{1}D and 1s²2p ($^{2}P_{3/2}^{\circ}$)4p ^{1}D levels, the experimental data of Kramidal et al.[10], are $E_{m} = E_{3} = 4.55365$ (m=3) and $E_{q} = E_{4} = 5.386143$ (q=4) in Rydberg. NIST gives us the limit energy, $E_{\infty} = 6.429778$ Ry. In this case, using Eq. (11), we find $\sigma_{1} = 2.982106$ and $\sigma_{2} = -0.273731$.

> For the triplets $1s^2 2p ({}^2P^0) ns {}^3P_0^0$ levels

$$E_{n} = E_{\infty} - \frac{1}{n^{2}} \left\{ Z - \sigma_{1} - \frac{\sigma_{2}}{n} - \sigma_{2} \times (n - m) \times (n - q) \times \left[\frac{\sigma_{2} \times S \times (S + 1)}{(n + m + q - s)^{3}} + \frac{\sigma_{2} \times S \times (n - m)}{(n - m + q)^{4}} + \frac{\sigma_{2} \times S \times (n + m)^{2}}{(n + m - q + s)^{5}} \right] \right\}_{(12)}^{2}$$

Using the exprimental data of Kramidal et al.[10], we obtain for the state $1s^22p$ ($^2P^{\circ}$)3s $^3P^{\circ}_{o}$ and $1s^22p$ ($^2P^{\circ}$)4s $^3P^{\circ}_{o}$ respectively $E_m = E_3 = 4.240051$ (m=3) and $E_q = E_4 = 5.266739$ (q=4). Energy limit is given by NIST data, we find $E_{\infty} = 6.42918875$ Ry. Using these data, eq. (12) gives : $\sigma_1 = 3.065447$ and $\sigma_2 = -1.512504$.

> For the triplets $1s^22p$ (²P^o)ns ³P₁⁰ levels

$$E_n = E_{\infty} - \frac{1}{n^2} \left\{ Z - \sigma_1 - \frac{\sigma_2}{n} - \sigma_2 \times (n - m) \times (n - q) \times \left[\frac{\sigma_2 \times S}{(n + q - s)^3} + \frac{\sigma_2 \times S \times (n - m)}{(n + m - s)^4} + \frac{S}{(n + s)^5} \right] \right\}_{(13)}^2$$

From the exprimental data of Kramidal et al.[10], we obtain for the $1s^22p$ (${}^{2}P^{o}$)3s ${}^{3}P^{o}_{1}$ and $1s^22p$ (${}^{2}P^{o}_{1/2}$)4s ${}^{3}P^{o}_{1}$, $E_m = E_3 = 4.240773$ (m=3) and $E_q = E_4 = 5.267537$ (q = 4). From NIST, we find $E_{\infty} = 6.429188$ Ry. We find then using eq. (13), we obtain $\sigma 1 = 3.069173531$ and $\sigma 2 = -1.521486$.

For the triplets $1s^22p ({}^2P_{3/2}^0)ns {}^3P_2^0$ levels

$$E_{n} = E_{\infty} - \frac{1}{n^{2}} \left\{ Z - \sigma_{1} - \frac{\sigma_{2}}{n} - \sigma_{2} \times (n - m) \times (n - q) \times \left[\frac{\sigma_{2} \times S}{(n + q + 3s)^{3}} - \frac{\sigma_{2} \times (S + 1)}{(n - m + 7s)^{4}} + \frac{S \times (n - m)}{(n + q - m)^{4}} \right] \right\}^{2}$$

$$= E_{\infty} - \frac{1}{n^{2}} \left\{ Z - \sigma_{1} - \frac{\sigma_{2}}{n} - \sigma_{2} \times (n - m) \times (n - q) \times \left[\frac{\sigma_{2} \times S}{(n + q + 3s)^{3}} - \frac{\sigma_{2} \times (S + 1)}{(n + q - m)^{4}} \right] \right\}^{2}$$

$$= E_{\infty} - \frac{1}{n^{2}} \left\{ Z - \sigma_{1} - \frac{\sigma_{2}}{n} - \frac{\sigma_{2} \times (n - m)}{(n + q - m)^{4}} \right\}^{2}$$

$$= E_{\infty} - \frac{1}{n^{2}} \left\{ Z - \sigma_{1} - \frac{\sigma_{2}}{n} - \frac{\sigma_{2} \times (n - m)}{(n + q - m)^{4}} \right\}^{2}$$

$$= E_{\infty} - \frac{1}{n^{2}} \left\{ Z - \sigma_{1} - \frac{\sigma_{2}}{n} - \frac{\sigma_{2} \times (n - m)}{(n + q - m)^{4}} \right\}^{2}$$

For the $1s^22p$ ($^2P^\circ$)3s $^3P_2^\circ$ and $1s^22p$ ($^2P^\circ$)4s $^3P_2^\circ$ levels, the exprimental data of Kramidal et al.[10]are $E_m = E_3 = 4.242282$ (m=3) and $E_q = E_4 = 5.269043$ (q=4) in Rydberg. Thus NIST databasegives us the limit energy, $E_\infty = 6.42918875$ Ry. In this case, Eq. (14) gives $\sigma_1 = 2.075764$ and $\sigma_2 = -1.536667$.

Resultats and Discusssions:-

Analysis of the present results is achieved in the framework of the standard quantum-defect δ theory and of the procedure by calculating the effective charge Z^{*} .

The relationship between Z^* and \Box is in the form:

$$Z^* = \frac{Z_{core}}{\left(1 - \frac{\delta}{n}\right)}$$
(15)

 $\begin{cases} Z^* \ge Z_{core} & if \quad \delta \ge 0\\ Z^* \prec Z_{core} & if \quad \delta \prec 0\\ \lim Z^* = Z_{core} \\ n \to \infty \end{cases}$

According to this equation, each Rydberg series must satisfy the following conditions : (16)

Our results are in perfect agreement with the avalaible theoretical and experimental values. For the N³⁺ ions, Z_{core} is directly obtain via the photoionization process of eq.(6) that gives : $N^{3+} + h\nu \rightarrow N^{4+} + e^{-} = Z_{core} = 4$ (17)

The present results are listed in tables 1-7 and compared with other avalaible theoretical calculations and experimental data. (17)

In **Table 1** we present the MAOT resonance energies (E) and quantum defect (δ) of the 1s²2p (²P^o_{3/2})ns ¹P Rydberg series relative to the ground state of the N³⁺ions. For this Rydberg series, we calculated the energies of the first Eighteen resonant states. We compared our results with the theoretical calculations of Liang et al.[9] and the experimental data of Kramidal et al. [10]. All our results are obtained empirically using equation (8). The comparison shows very good agreement. We also note that the quantum defect $\delta > 0$ and decreases as the principal quantum number increases. Thus up to n = 5, the comparison shows that the $|\Delta E|$ energy differences from experimental data are less than 0.005. For n = 6 up to n = 15, our results are only compared with R-Matrix theoretical calculations of Liang et al.[9] and comparison is considered very satisfactory. Thus, for this Rydberg series, we can expect our results up to n = 20 to be accurate.

In **Table 2** we present the MAOT resonance energies (E) and quantum defect (δ) of the 1s²2p (²P^o_{3/2})nd ¹P Rydberg series relative to the ground state of the N³⁺ ions. Our results are compared with those of Liang et al. [9] and the experimental data of Kramidal et al. [10]. Liang et al. [9] used the R-Matrix method to calculate energies from n = 5 up to n = 15. All our results are obtained empirically using eq. (9). Thus, up to n = 10, comparison shows very good agreement and the $|\Delta E|$ energy differences are less than 0.0001 Ryd. Thus, for this Rydberg series, the comparison is considered very satisfactory, and we can expect our results to be accurate up to n = 20.

In **Table 3**, we show a comparison of the resonance energies (E) and quantum defect (δ) of the 1s²2p (²P^o_{1/2})np ¹P Rydberg series. The MAOT energy positions are calculated from eq. (10). The agreements between the studies are very good, and the quantum defect is practically decreasing throughout the series. The comparison shows that the energy differences from experimental data are less than 0.001 Ry.

Agreement between MAOT results and experimental data is very good. We can therefore expect our results up to n = 20 to be accurate.

Table 4 shows the resonance energies and quantum defects of the singlets $1s^22p ({}^2P^o_{3/2})np {}^1D$ Rydberg series states from the ground state of the N³⁺ ions. For this Rydberg series, we also calculated the energies of the first eighteen resonant states. We note that the quantum defect decreases as the principal quantum number increases. The comparison shows that the [ΔE]energy differences from experimental data are less than 0.001 eV. Thus, for this Rydberg series, the comparison is considered very satisfactory, and we can expect our results n > 11 to be accurate.

We present in **Table 5** the MAOT resonance energies (E) and quantum defect (δ) of the triplets $1s^22p$ (²P^o)ns ³P₀Rydberg series relative to the ground state of the N³⁺ ions. We only compared our results with those of Kramidal et al. [10]. All our results are calculated empirically using equation (12). The comparison shows very good agreement. The [Δ E]energy differences from experimental data are less than 0.0001 Ry. Thus, for this Rydberg series, the comparison is considered very satisfactory, and we can expect our results to be accurate up to n = 20.

In **Table 6**, we show a comparison of the resonances energies (E) and quantum defect (δ) of the triplets $1s^22p$ (²P^o)ns ³P₁ Rydberg series to the ground state of the N³⁺. The present energy positions are calculated from eq. (13). The agreement between the studies are very good, and the quantum defect is practically decreasing throughout the series. Agreement between MOAT results and experimental data is very good. We can therefore expect our results

up to n = 20 to be accurate. The comparison shows that the [ΔE]energy differences from experimental data are less than 0.0001 Ry.

In **Table 7** we present the MAOT resonance energies (E) and quantum defect (δ) of the triplets $1s^22p$ (²P^o)ns ³P₂Rydberg series relative to the ground state of the N³⁺ ion. We compared our results with those of Kramidal et al. [10]. All our results are calculated empirically using eq. (14). The comparison shows very good agreement. We also note that the quantum defect decreases as the principal quantum number increases. The comparison shows that the [Δ E] energy differences from experimental data are less than 0.0001 Ry. Thus, for this Rydberg series, the comparison is considered very satisfactory, and we can expect our results to be accurate up to n = 20.

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

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

Table 1:- Resonance energies (E_n, Ry) and quantum defect δ of the singlet $1s^22p$ ($^2P^{o}_{3/2}$)ns 1P Rydberg series of the N IV. The resultats are expressed in Rydberg (Ry). The MAOT present results compared with the R-matrix method of Liang et al.[9] and the NIST data [10]. (1 Ry = 0.5 a.u = 13.605698 eV).

$1s^{2}2p ({}^{2}P_{3/2})ns {}^{4}P$						
E(Ry)					δ	
n	МАОТ	R- MATRIX	NIST	$ \Delta E $	МАОТ	
3	4.310560		4.310560	0.000	0.25	
4	5.292799		5.292799	0.000	0.25	
5	5.722551	5.72038	5.727741	0.005	0.24	
6	5.947952	5.94535			0.24	
7	6.080629	6.07802			0.23	
8	6.165236	6.16274			0.22	
9	6.222464	6.22012			0.21	
10	6.262961	6.26076			0.21	
11	6.292663	6.29060			0.20	
12	6.315090	6.31315			0.19	
13	6.332437	6.33061			0.18	
14	6.346128	6.34440			0.17	
15	6.357123	6.35548			0.16	
16	6.366086				0.15	
17	6.373487				0.14	
18	6.379671				0.13	
19	6.384888				0.12	
20	6.389332				0.11	
1						
80	6 429778					

 $|\Delta E|$: is energy differences relative to the experimental data.

Table 2:- Resonance energies (E_n , Ry) and quantum defect δ of the singlets $1s^22p$ (${}^2P_{3/2}^{\circ}$)nd 1P Rydberg series of the N IV. The resultats are expression in Rydberg (Ry). The MAOT present results are compared with the R-matrix results of Liang et al. [9] and the NIST data of Kramidal et al.[10]. (1 Ry = 0.5 a.u = 13.605698 eV). $1s^22p$ (${}^2P_{2}^{\circ}$) nd 1P

15 2p (1	3/2)110					
n	МАОТ	R-MATRIX	NIST	$ \Delta E $	δ MAOT	
n	MAOT	R-MATRIX	NIST	ΔE	МАОТ	

5	5.79991	5.80101	5.79991	0.00000	-0.040
6	5.99060	5.99114	5.99060	0.00000	-0.035
7	6.10622	6.10646	6.10627	0.00005	-0.032
8	6.18154	6.18162	6.18163	0.00009	-0.028
9	6.23332	6.23329	6.23320	0.00012	-0.024
10	6.27044	6.27032	6.27037	0.00007	-0.021
11	6.29795	6.29775			-0.017
12	6.31890	6.31864			-0.013
13	6.33523	6.33492			-0.009
14	6.34820	6.34784			-0.005
15	6.35868	6.35827			-0.001
16	6.36726				0.003
17	6.37437				0.006
18	6.38034				0.011
19	6.38539				0.015
20	6.38970				0.019
1					
∞	6.429778				

Table 3:- Resonance energies (E_n , Ry) and quantum defect δ of the singlets $1s^22p ({}^2P^{o}_{1/2})np {}^1P$ Rydberg series of the N IV. The resultats are expression in Rydberg (Ry). The MAOT present results are only compared with the avalaible NIST data [10]. (1 Ry = 0.5 a.u = 13.605698 eV).

$1s^{-}2p(P_{1/2})np^{-}$	P				
E(Ry)				δ	
n	МАОТ	NIST	$ \Delta E $	МАОТ	
3	4.38239	4.38239	0.00000	0.20	
4	5.327829	5.327829	0.00000	0.18	
5	5.739685	5.739573	0.00011	0.18	
6	5.956290	5.956314	0.00002	0.17	
7	6.084420	6.084520	0.00001	0.17	
8	6.166559	6.16602	0.00054	0.17	
9	6.222389			0.16	
10	6.262067			0.16	
11	6.291275			0.16	
12	6.313397			0.15	
13	6.330551			0.15	
14	6.344118			0.14	
15	6.355033			0.13	
16	6.363943			0.12	
17	6.371309			0.11	
18	6.377469			0.10	
19	6.3826706			0.09	
20	6.3871031			0.08	
1					
∞	6.427421				

 $[\Delta E]$ is energy differences relative to the experimental data.

Table 4:- Resonance energy (E_n, Ry) and quantum defect δ determined of the singlets $1s^22p ({}^2P^o{}_{1/2})np {}^1D$ Rydberg series of the N³⁺. The resultats are expression in Rydberg (Ry). The MAOT present results are compared with the NIST experimental data[10]. (1 Ry = 0.5 a.u = 13.605698 eV).

$1s^22p$	$(^{2}P^{o})ns$	$^{3}P_{0}$

n	ΜΑΟΤ	NIST	$ \Delta E $	МАОТ
3	4.240051	4.240051	0.000	0.11
4	5.266739	5.266739	0.000	0.12
5	5.709061	5.757200	0.048	0.12
6	5.939919	5.937726	0.001	0.12
7	6.075334	6.07230	0.003	0.13
8	6.161457	6.15799	0.003	0.13
9	6.219592	6.21775	0.002	0.14
10	6.260669	6.25902	0.002	0.14
11	6.290763			0.14
12	6.313467			0.15
13	6.331015			0.16
14	6.344858			0.16
15	6.355970			0.16
16	6.365025			0.17
17	6.372500			0.17
18	6.378743			0.17
19	6.384010			0.18
20	6.388495			0.18
1				
∞	6.42918875			

Table 5:- Resonance energies (E_n, Ry) and quantum defect δ of the tripets $1s^22p$ (²P^o)ns ³P₀ Rydberg serie of the N IV. The MAOTresults are calculated in Rydberg (Ry) and compared with the experimental data of NIST[10]. (1 Ry = 0.5 a.u = 13.605698 eV).

$1s^{2}2p (^{2}P^{o}_{1/2})np ^{1}D$				
E(Ry)				δ
n	МАОТ	NIST	$\left \Delta E\right $	МАОТ
3	4.553655	4.55365	0.0000	0.07
4	5.386143	5.386143	0.0000	0.08
5	5.766305			0.08
6	5.971087	5.971388	0.0003	0.09
7	6.093857	6.094130	0.0003	0.09
8	6.173207	6.173458	0.0002	0.10
9	6.227433	6.227598	0.0002	0.10
10	6.266124	6.266140	0.0000	0.11
11	6.294693	6.294764	0.0001	0.11
12	6.316386			0.12
13	6.333244			0.12
14	6.346604			0.13
15	6.357371			0.13
16	6.366175			0.14
17	6.373466			0.14
18	6.379571			0.15
19	6.384735			0.15
20	6.389141			0.16
1				
∞	6.429778			

 $[\Delta E]$ is energy differences relative to the experimental data

$1s^{2}2p (^{2}P^{0})ns^{-1}$	³ P ₁				
E(Ry)				δ	
n	МАОТ	NIST	$ \Delta E $	МАОТ	
3	4.240773	4.240773	0.0000	0.29	
4	5.267537	5.267537	0.0000	0.29	
5	5.708603	5.708590	0.0000	0.29	
6	5.938741	5.938470	0.0003	0.29	
7	6.073978	6.073214	0.0008	0.29	
8	6.160171	6.15883	0.0013	0.29	
9	6.218460	6.21819	0.0003	0.29	
10	6.259706	6.25934	0.0004	0.28	
11	6.289956			0.28	
12	6.312794			0.27	
13	6.330455			0.27	
14	6.344392			0.26	
15	6.355581			0.26	
16	6.364699			0.25	
17	6.372227			0.24	
18	6.378513			0.23	
19	6.383815			0.22	
20	6.388329			0.21	
:					
00	6.42918875				

Table 6:- Resonance energies (E_n, Ry) and quantum defect δ of the triplets $1s^22p$ $(^2P^o)ns$ 3P_1 Rydberg series of the N IV. The MAOT results are calculated in Rydberg (Ry) for direct comparison with the experimental data of NIST [10]. (1 Ry = 0.5 a.u = 13.605698 eV).

Table 7:- Resonance energies (E_n , Ry) and quantum defect δ of the triplets $1s^22p$ ($^2P^o$)ns 3P_2 Rydberg series of the N³⁺. All results are in Rydberg (Ry). The MAOT present results are compared with the only experimental data NIST[10]. (1 Ry = 0.5 a.u = 13.605698 eV).

$1s^{2}2p (^{2}P^{0})ns$	³ P ₂				
E(Ry)				δ	
n	МАОТ	NIST	$ \Delta E $	МАОТ	
3	4.242282	4.242282	0.00000	0.29	
4	5.269043	5.269043	0.00000	0.29	
5	5.710101	5.710108	0.00007	0.28	
6	5.940258	5.940184	0.00007	0.28	
7	6.075413	6.075102	0.00031	0.27	
8	6.161462	6.160992	0.00054	0.27	
9	6.219591	6.219077	0.00051	0.26	
10	6.260682	6.259984	0.00069	0.25	
11	6.290794			0.25	
12	6.313513			0.24	
13	6.331073			0.23	
14	6.344925			0.22	
15	6.356042			0.21	
16	6.365101			0.20	
17	6.372578			0.19	
18	6.378822			0.18	
19	6.384087			0.16	

20		6.388571	0.15
	1		
c	x	6.42918875	

Conclusion:-

In short, energy position in the photoionization of the N IV from the ground state of the the $1s^22p(^2P)ns^{1}P$, $1s^22p(^2P)ns^{1}P$, $1s^22p(^2P_{3/2})np^{1}D$ and $1s^22p(^2P^{\circ})ns^{-3}P_{0,1,2}$ Rydberg series are reported using the Modified Atomic Orbital Theory (MAOT) semi-empirical procedure. The simplicity of the semi-empirical MAOT procedure has allowed us to calculate precise values of energies without having to resort either to a complex mathematical formalism or to a specific calculation code via a computer program. We find that our results are in good agreement with the available expression data and latest theoretical resultats...This work may be of interest for future experimental and theoretical studies in the photoabsorption spectrum of N³⁺.

Acknowledgments:-

The authors are grateful to the Orsay Institute of Molecular Sciences (OIMS), Paris, France and the Abdus Salam International Center for Theoretical Physics (ICTP), Trieste, Italy.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

CrediT Author Statement,

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

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

Ndeye Astou THIAM: Reviewing; Formal analysis, Validation.

Sory DIAW: Reviewing; Formal analysis, Validation.

Omar Baba DIA: Reviewing; Formal analysis, Validation.

Papa Mamadou NDIAYE [;] Reviewing: ;Formal analysis, Validation.

Cheikh Tidiane DIOUF : Reviewing; Formal analysis, Validation.

References:-

[1]: Bregman J. N and J. P. Harrington, Astrophys. Journal . 309, 833 (1986).

https://doi.org/10.1086/164652

[2] : Hofmann I, Laser Part. Beams 8, 527 (1990). https://doi.org/10.1017/S026303460000896X

[3] :Berrington K, Quigley L and Zhang HL. The calculation of high-energy photoionization cross

sections for the Be isoelectronic sequence. J. Phys. B: At. Mol. Opt. Phys. 1997:30; 5409–5417.

[4] : Garcia J, Kallman TR, Witthoeft M, Behar E, Mendoza C, Palmeri P, Quinet P, Bautista MA and Klapisch M. NITROGEN K-SHELL PHOTOABSORPTION. The Astrophysical Journal Supplement Series 2009:185;477–485.

[5] : Sakho I (2013) Photoabsorption of H- and He via the Modified Atomic Orital Theory : Application to the 1P0 – Rydberg states. Chin. J. Phys. 51, 209.

[6]: Diop B, Faye M, Dieng M, Sow M, Gueye M et al (2014). Modified Atomic Orbital Study of Dominant Rydberg series in the photoionization spectra of halogen- like Kr+ and Xe+ ions. Chin. J. Phys. 52, 1227-1237.

[6] :Sow, M., Ndoye, F., Traoré, A., Diouf, A., Sow, B., Gning, Y. and Diagne, P.A.L. (2021) Photoionization Study of the 2 s22p2(1D)ns(2D), 2s22p2(1D)nd(2P), 2s 22p 2(1D)nd(2S), 2s 22p 2(1S) nd 2D and 2s 22p3(3P)np(2D) Rydberg Series of O+ Ions via the Modified Atomic Orbital Theory.Journal of Modern Physics, 12, 1375-1386. https://doi.org/10.4236/jmp.2021.1210086

[7]: Sow M, Dieng M, Tine M, Faye M, Diop B et al (2014), calculations of high lying (2pns) 1,3P0 and (2pnd) 1,3P0 Rydberg states of Be atom via the Modified Atomic Orbital Theory . Chin. J. Phys. 52, 1459...

[8] : Sow M, Ndoye F, Diop B, Traoré A, Diouf A, Sow B, 'Modified Atomic Orbital Theory of the O+ ion Originating from 2D0 and 4S0 Metastable States'' Journal of Applied Mathematics and Physics, (2022), 10, 1873-1886

[9] :Liang, L., & Zhou, C. (2018). K-shell photoionization of Be-like nitrogen from the ground state: energies and Auger widths of the high-lying double-excited states for N IV. Canadian Journal of Physics, 96(11), 1183-1191. [10] :Kramida, A., Ralchenko, Yu., Reader, J., et NIST ASD Team (2023). Base de données NIST Atomic Spectra (ver. 5.11), [En ligne]. Disponible : https://physics.nist.gov/asd [2024, 11 septembre]. Institut national des normes et de la technologie, Gaithersburg, MD. DOI : https://doi.org/10.18434/T4W30F.