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Modified Atomic Orbital Theory of the O^+ Ion Originating from $2D^0$ and $4S^0$ Metastable States

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Abstract

We report in this paper energy positions of the $2D^0\_2s^22p^2(^1D)nd(^2F)$; $2D^0\_2s^22p^2(^1D)nd(^2D)$; $2D^0\_2s^22p^2(^1D)nd(^2P)$; $2D^0\_2s^22p^2(^1D)ns(^2D)$; $2D^0\_2s^22p^3(^3D)np(^2P)$; $2D^0\_2s^22p^3(^3D^0)np(^2F)$, and $4S^0\_2s^22p^3(^5S^0)np(^4P)$ Rydberg series in the photoionization spectra originating from $2D^0$ and $4S^0$ metastable states of O^+ ion. Calculations are performed up to $n = 20$ using the Modified Orbital Atomic Theory (MAOT) [1]. The present results are compared to the experimental data of Aguilar *et al.* [2] 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.

Keywords

Semiempirical Calculations, Modified Orbital Atomic Theory, Electron Correlation Calculations, Atoms and Ions, Rydberg Series, Quantum Defect

1. Introduction

Ion escape is of particular interest for studying the evolution of the atmosphere on geological time scales. From this study, we suggested that O^+ ions observed in the plasma mantle and cusp have enough energy and velocity to escape the magnetosphere and are lost into the solar wind or in the distant magnetotail. Thus, this study aims to investigate Rydberg series of O^+ ions for which photoabsorption from low-lying metastable states of open-shell ions has been shown to be important in laboratory and astrophysical plasmas [3] [4] [5]. Quantitative and qualitative measurements of photoionization of ions provide precision data on ionic structure, and guidance to the development of theoretical approaches of multielectron interactions. Thus, Aguilar *et al.* [2] performed the first experiment on the Absolute photoionization of O^+ by using the merged-beam tech-

nique above the first ionization threshold at the Advanced Light Source (ALS).

For comparison with high-resolution measurements, state-of the-art-theoretical methods are required using highly correlated wave functions including relativistic effects [6]. Among the *ab initio* methods applied in the photoionization studies of atoms and ions are the Hartree-Fock multi-configurationnal (MCDF) method [7], the Quantum Defect Theory [8], the R-matrix approach [9] widely used for international collaborations such as the Opacity Project [4], the Multi-Configuration Dirac-Hartree-Fock method (MCDHF) [10], in the form of the grasp2k relativistic atomic structure package [11]. The MCDHF has been used to compute with high precision the 2^3P_1–2^3P_0 separation energy, including relativistic contributions to electron-electron correlations and radiative corrections.

In the present paper, we intend to provide accurate data on the photoionization of O^+ ion from $2D^0$ *and* $4S^0$ metastable states that may be useful guideline for the physical atomic community. In addition, we aim to demonstrate the possibilities to use the Modified Atomic Orbital Theory semi-empirical procedure [1] [12] [13] to reproduce excellently experimental data from merged beam facilities. For this purpose, we report calculations of energy resonances of the $2D^0\_2s^22p^2(^1D)nd(^2F)$; $2D^0\_2s^22p^2(^1D)nd(^2D)$; $2D^0\_2s^22p^2(^1D)nd(^2P)$; $2D^0\_2s^22p^2(^1D)ns(^2D)$; $2D^0\_2s^22p^3(^3D)np(^2P)$; $2D^0\_2s^22p^3(^3D^0)np(^2F)$, *and* $4S^0\_2s^22p^3(^5S^0)np(^4P)$ Rydberg series in the photoionization spectra originating from $2D^0$ and $4S^0$ metastable states of O^+ ion. Calculations are performed using the *MAOT* method [14] [15] and analysis of the data tabulated is achieved via the MAOT procedure along with the quantum defect theory.

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 experimental data of Aguilar *et al*. [2]. In Section 4, we summarize our study and draw conclusions.

2. Theory

2.1. Brief Description of the MAOT Formalism

In the framework of Modified Atomic Orbital Theory (MAOT), total energy of $(n\ell)$-given orbital is expressed in the form [13] [16].

$$E(n\ell) = -\frac{\left[Z-\sigma(\ell)\right]^2}{n^2} \tag{1}$$

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

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

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

$$E = -\sum_{i=1}^{M} \frac{\left[Z - \sigma_i \left({}^{2S+1}L^{\pi} \right) \right]^2}{\upsilon_i^2} \tag{2}$$

In the photoionisation study, energy resonances are generally measured relatively to the $E\infty$ converging limit of a given $({}^{2S+1}L_J)$ *nl*-Rydberg series. For these states, the general expression of the energy resonances is given by the formula of Sakho presented previously [17] (in Rydberg units):

$$\begin{aligned} E_n = E_\infty - \frac{1}{n^2} \Bigg\{ & Z - \sigma_1 \left({}^{2S+1}L_J \right) - \sigma_2 \left({}^{2S+1}L_J \right) \times \frac{1}{n} \\ & - \sigma_2^{\mu} \left({}^{2S+1}L_J \right) \times (n-m) \times (n-q) \sum_k \frac{1}{f_k(n,m,q,s)} \Bigg\}^2 \end{aligned} \tag{3}$$

In this equation m and q $(m < q)$ denote the principal quantum numbers of the $({}^{2S+1}L_J)$ *nl*-Rydberg series of the considered atomic system used in the empirical determination of the $\sigma_i({}^{2S+1}L_J)$-*s*creening constants, s represents the spin of the *nl*-electron ($s = 1/2$), E_∞ is the energy value of the series limit generally determined from the NIST atomic database, E_n denotes the corresponding energy resonance, and Z represents the nuclear charge of the considered element. The only problem that one may face by using the MAOT formalism is linked to the determination of the $\sum_k \frac{1}{f_k(n,m,q,s)}$ term. The correct expression of this term is determined iteratively by imposing general Equation (3) to give accurate data with a constant quantum defect (δ) values along all the considered series. The value of μ is fixed to 1 and 2 during the iteration. The quantum defect (δ) is calculated from the standard formula below

$$E_n = E_\infty - \frac{RZ_{core}^2}{(n-\delta)^2} \Rightarrow \delta = n - Z_{core}\sqrt{\frac{R}{E_\infty - E_n}} \tag{4}$$

In this equation, R is the Rydberg constant, E_∞ denotes the converging limit, Z_{core} represents the electric charge of the core ion, and (δ) means the quantum defect.

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 $Z_{core} = p + 1$.

In addition, theoretical and measured energy positions can be analyzed by calculating the Z^* effective charge in relationship with the quantum defect (δ).

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

$$Z^* = \frac{Z_{core}}{1 - \frac{\delta}{n}} \tag{5}$$

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

$$\begin{cases} Z^* \geq Z_{core} & \text{if } \delta \geq 0 \\ Z^* \leq Z_{core} & \text{if } \delta \prec 0 \\ \lim_{n\to\infty} Z^* = Z_{core} \end{cases} \quad (6)$$

2.2. Energy Positions of the $2D^0\_2s^22p^2(^1D)nd(^2F)$; $2D^0\_2s^22p^2(^1D)nd(^2D)$; $2D^0\_2s^22p^2(^1D)nd(^2P)$; $2D^0\_2s^22p^2(^1D)ns(^2D)$; $2D^0\_2s^22p^3(^3D)np(^2P)$; $2D^0\_2s^22p^3(^3D^0)np(^2F)$, Rydberg Series from $2D^0$ Metastable State

Using Equation (3) we find

- **For $2D^0\_2s^22p^2(^1D)nd(^2F)$ levels**

$$E_n = E_\infty - \frac{1}{n^2}\left\{Z - \sigma_1 - \frac{\sigma_2}{n} + \sigma_2 \times (n-m) \times (n-q) \times \left[\frac{1}{(n+q-s)^2} + \frac{1}{(n+m-s)^3} + \frac{1}{(n+m-s)^4} + \frac{1}{(n+q-m+s)^5}\right]\right\}^2 \quad (7)$$

Using the experimental data of ALS [9], we obtain (in eV) E_5 = 32.044 ± 0.20 (m = 5) and E_6 = 32.753 ± 0.20 (q = 6) respectively for the $2D^0\_2s^22p^2(^1D)5d(^2F)$ and $2D^0\_2s^22p^2(^1D)6d(^2F)$ levels. From NIST [18], we find E_∞ = 34.311 eV. Using these data, Equation (7) gives σ_1 = 6.022617664 ± 0.333296261 *and* σ_2 = −0.317908474 ± 0.012159751

- **For $2D^0\_2s^22p^2(^1D)nd(^2D)$ levels:**

$$E_n = E_\infty - \frac{1}{n^2}\left\{Z - \sigma_1 - \frac{\sigma_2}{n} + \sigma_2 \times (n-m) \times (n-q) \times \left[\frac{1}{(n+m-s)(n+q-s)^2} + \frac{1}{(n-s)^3}\right]\right\}^2 \quad (8)$$

For the $2D^0\_2s^22p^2(^1D)5d(^2D)$ and $2D^0\_2s^22p^2(^1D)6d(^2D)$ levels, we find using the experimental data of ALS *et al.* [2], E_5 = 32.083 ± 0.20 (m = 5) and E_6 = 32.775 ± 0.20 (q = 6). From NIST [18], we find E_∞ = 34.311 eV. Equation (8) provides then σ_1 = 6.020774511 ± 0.335007227 *and* σ_2 = −0.220533344 ± 0.012205725

- **For $2D^0\_2s^22p^2(^1D)nd(^2P)$ levels**

$$E_n = E_\infty - \frac{1}{n^2}\left\{Z - \sigma_1 - \frac{\sigma_2}{n} + \sigma_2 \times (n-m) \times (n-q) \times \left[\frac{1}{(n+q-s)^3} + \frac{1}{(n+q+s-m)^4} + + \frac{1}{(n+q-m+3s)^5}\right]\right\}^2 \quad (9)$$

For the $2D^0\_2s^22p^2(^1D)5d(^2P)$ *and* $2D^0\_2s^22p^2(^1D)6d(^2P)$ levels the experimental energy positions ALS *et al.*, [2] are, E_5 = 32.107 ± 0.20 (m = 5) *and* E_6 = 32.786 ± 0.20 (q = 6). From NIST [18], we find E_∞ = 34.311 eV. In that case, we find using Equation (9) σ_1 = 6.009528595 ± 0.472635519 *and* σ_2 = −0.109667938

± 0.020784332

- **For $2D^0\_2s^22p^2(^1D)ns(^2D)$ levels**

$$E_n = E_\infty - \frac{1}{n^2}\left\{Z - \sigma_1 - \frac{\sigma_2}{n} + \sigma_2 \times (n-m)\times(n-q) \times\left[\frac{1}{(n+q-m+s)} + \frac{1}{(n-s)^2(n+2m-q)^3}\right]\right\}^2 \quad (10)$$

From ALS of Aguilar *et al.* [2], we obtain for the $2D^0\_2s^22p^2(^1D)6s(^2D)$ *and* $2D^0\_2s^22p^2(^1D)7s(^2D)$ E_6= 32.267 ± 0.20 (m = 6) *and* E_7 = 32. 881 ± 0.20 (q = 7). From NIST [18], we find E_∞ = 34.311 eV. We find then using Equation (10) σ_1 = 6.067877676 ± 0.430724379 *and* σ_2 = −2.360746016 ± 0.19010132

- **For $2D^0\_2s^22p^3(^3D)np(^2P)$ levels**

$$E_n = E_\infty - \frac{1}{n^2}\left\{Z - \sigma_1 - \frac{\sigma_2}{n} + \sigma_2 \times (n-m)\times(n-q) \times\left[\frac{1}{(n+q-s)^2(n+s-m)^2} + \frac{1}{(n+s-m)^3} + \frac{1}{(n+q+s-m)^4}\right]\right\}^2 \quad (11)$$

From ALS *et al.* [2], we obtain for the $2D^0\_2s^22p^3(^3D)3p(^2P)$ *and* $2D^0\_2s^22p^3(^3D)4p(^2P)$ E_3= 37.604 ± 0.20 (m = 3) *and* E_4 = 42.149 ± 0.20 (q = 4). From NIST [18], we find E_∞ = 46.707 eV. *We find then using* Equation (11) σ_1= 6.100874328 ± 0.092439223 *and* σ_2 = −1.664259453 ± 0.207487744

- **For $2D^0\_2s^22p^3(^3D^0)np(^2F)$ levels**

$$E_n = E_\infty - \frac{1}{n^2}\left\{Z - \sigma_1 - \frac{\sigma_2}{n} + \sigma_2 \times (n-m)\times(n-q) \times\left[\frac{1}{(n+q-s)^2} + \frac{1}{(n+s-m)^2} - \frac{1}{(n+s-m)^3}\right]\right\}^2 \quad (12)$$

From ALS *et al.* [2], we obtain for the $2D^0\_2s^22p^3(^3D^0)3p(^2F)$ *and* $2D^0\_2s^22p^3(^3D^0)4p(^2F)$ E_3= 38.686 ± 0.20 (m = 3) *and* E_4 = 42.409 ± 0.20 (q = 4). From NIST [18], we find E_∞ = 46.620 eV. *We find then using* Equation (12) σ_1 = 5.971438364 ± 0.124812413 *and* σ_2 = −0.787027868 ± 0.028785514

2.3. Energy Positions of the $4S^0\_2s^22p^3(^5S^0)np(^4P)$ Rydberg Series from $4S^0$ Metastable State

Using Equation (3), energy positions of the $4S^0\_2s^22p^3(^5S^0)np(^4P)$ prominent Rydberg series from $4S^0$ metastable state of O^+ are given by (in Rydberg units)

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

From ALS *et al.* [2], we obtain for the $4S^0\_2s^22p^3(^5S^0)4p(^4P)$ *and* $4S^0\_2s^22p^3(^5S^0)5p(^4P)$ $E_4 = 38.216 \pm 0.20$ ($m = 4$) *and* $E_5 = 39.919 \pm 0.20$ ($q = 5$). From NIST [18], we find $E_\infty = 42.586$ eV. We find then using Equation (13) $\sigma_1 = 5.99920618 \pm 0.207827476$ *and* $\sigma_2 = -1.0645904 \pm 0.429419911$.

3. Results and Discussions

The results obtained in the present paper are listed in Tables 1-7 and compared with the Advaced Light Source experimental data of Aguilar *et al.* [2].

In Table 1, we quote the present *MAOT* results for energy resonances (E) and quantum defect (δ) of the $2D^0 2s^2 2p^2(^1D)nd(^2F)$ Rydberg series relatively to the $2D^0$_metastable state of O^+ ion. The current energy positions are calculated from Equations (5) along with $Z = 8$, $m = 5$, *and* $q = 6$, $\sigma_1 = 6.022617664 \pm 0.333296261$ and $\sigma_2 = -0.317908474 \pm 0.012159751$. All these screening constant are evaluated using the Advaced Light Source (ALS) experimental results of Aguilar *et al.* [2], and take from NIST [18] the E_∞ energy limits which is 34.311 eV. Then our results are converted into eV for direct comparison by using the infinite Rydberg

Table 1. Energy resonances (E) and quantum defect (δ) of the $2D^0 2s^2 2p^2(^1D)nd(^2F)$ Rydberg series observed in the photoionization spectra originating from the $2D^0$ metastable states of O^+. The present results (*MAOT*) are compared to the Advanced Light Source (ALS) of Aguilar *et al.* [2]. The results are expressed in eV. The energy uncertainties in the present calculations are indicated into parenthesis.

	$E(eV)$			δ	
n	*MAOT*	*ALS*	$\lvert\Delta E\rvert$	*MAOT*	*ALS*
5	32.044(200)	32.044	0.000	0.097	0.097
6	32.753(200)	32.753	0.000	0.084	0.084
7	33.175(150)	33.179	0.005	0.060	0.057
8	33.444(120)	33.448	0.004	0.059	0.046
9	33.629(110)	33.632	0.003	0.057	0.028
10	33.760(100)	33.763	0.003	−0.005	−0.008
11	33.857(87)	33.860	0.003	−0.005	−0.020
12	33.930(70)	33.933	0.003	−0.005	−0.045
13	33.989(55)	33.991	0.002	−0.005	−0.100
14	34.034(41)	34..036	0.002	−0.004	−0.142
15	34.070(30)	34.072	0.002	−0.004	−0.181
16	34.100(20)	34.102	0.002	−0.004	−0.249
17	34.126(11)	34.127	0.001	−0.004	−0.034
18	34.148(08)			−0.003	
19	34.167(05)			−0.004	
20	34.185(04)			−0.004	
⋮					
∞[a]	34.311				

[a]NIST atomic database [18]. |ΔE|: energy differences relative to the experimental data.

(1 Ry = 0.5 a.u = 13.605698 eV). It is seen that the data obtained compared very well to the experimental data of Aguilar *et al.* [2].

Up to n = 17, the maximum energy differences relative to the experimental data is less than 0.006 eV. In addition, Quantum defects are positive up to n = 9 because the effective charges of these self-ionizing states are less than the charge of the O^+ ion, and if not, they are negative from n = 10 *up to* n = 20. We also note that up to n = 9, the quantum defect of these resonant states decreases on average by 0.015 when the principal quantum number increases. *For* n = 10 *up to* n = 20, Quantum defects are almost constant. The agreements between the *MAOT* results and experimental data are seen to be very good and the quantum defect agrees well with the analysis condition of Equation (6). This allows us to expect our results on the resonance energies for this Rydberg series up to n = 20 to be accurate.

In Table 2, we compare the present *MAOT* energy resonances (E) and quantum defect (δ) of the $2D^0 2s^2 2p^2(^1D)nd(^2D)$ Rydberg series relatively to the $2D^0$_ metastable state of O^+ ion to experimental data [2]. All our energy values are

Table 2. Energy resonances (E) and quantum defect (δ) of the $2D^0 2s^2 2p^2(^1D)nd(^2D)$ Rydberg series observed in the photoionization spectra originating from the $2D^0$ metastable states of O^+. The present results (*MAOT*) are compared to the Advanced Light Source (ALS) of Aguilar *et al.* [2]. The results are expressed in eV. The energy uncertainties in the present calculations are indicated into parenthesis.

	$E(eV)$			δ	
n	*MAOT*	*ALS*	$\lvert\Delta E\rvert$	*MAOT*	*ALS*
5	32.083(200)	32.083	0.000	0.054	0.054
6	32.775(200)	32.775	0.000	0.042	0.042
7	33.195(194)			0.061	0.057
8	33.464(178)			0.048	0.046
9	33.649(161)			0.022	0.028
10	33.780(146)			−0.011	−0.008
11	33.877(130)			−0.012	−0.020
12	33.950(112)			−0.010	−0.045
13	34.009(99)			−0.012	−0.100
14	34.074(83)			−0.014	−0.142
15	34.090(72)			−0.011	−0.181
16	34.108(59)			−0.011	−0.249
17	34.141(48)			−0.012	−0.334
18	34.168(44)			−0.012	
19	34.187(39)			−0.012	
20	34.200(37)			−0.012	
⋮					
∞[a]	34.311				

[a]NIST atomic database [18]. $\lvert\Delta E\rvert$: energy differences relative to the experimental data.

obtained empirically using Equation (8) and converted into (eV) for direct comparison. Here again, the agreements are seen to be very good. Along the series, the quantum defect agrees well with the analysis condition of Equation (6). We also note that, the present quantum defect is almost constant for $n \geq 10$.

In Table 3, we show a comparison of the energy resonances (E) and quantum defect (δ) of the $2D^0 2s^2 2p^2(^1D)nd(^2P)$ Rydberg states relatively to the $2D^0$_metastable state of O^+ ion. The current energy positions are calculated from equations (9) along with $Z = 8$, $m = 5$, *and* $q = 6$, $\sigma_1 = 6.009528595 \pm 0.472635519$ *and* $\sigma_2 = -0.109667938 \pm 0.020784332$. The agreements between the *MOAT* results and experimental data are seen to be very good. Along all the series investigated, we note that, the quantum defect agrees well with the *MAOT* analysis condition of Equation (6). This may expect our results up to $n = 20$ to be accurate.

In Table 4, we list the present energy resonances (E) and quantum defect (δ) for the $2D^0 2s^2 2p^2(^1D)ns\,(^2D)$ Rydberg states relatively to the $2D^0$_metastable state of O^+ ion compared to the experimental data [2]. The current energy positions are calculated from Equations (10) along with $Z = 8$, $m = 6$, *and* $q = 7$, $E_\infty = 34.311$

Table 3. Energy resonances (E) and quantum defect (δ) of the $2D^0 2s^2 2p^2(^1D)nd(^2P)$ Rydberg series observed in the photoionization spectra originating from the $2D^0$ metastable states of O^+. The present results (MAOT) are compared to the Advanced Light Source (ALS) of Aguilar *et al.* [2]. The results are expressed in eV. The energy uncertainties in the present calculations are indicated into parenthesis.

	$E\,(eV)$			δ	
n	*MAOT*	*ALS*	$\lvert\Delta E\rvert$	*MAOT*	*ALS*
5	32.107(200)	32.107	0.000	0.028	0.028
6	32.786(200)	32.786	0.000	0.021	0.021
7	33.205(180)			0.054	0.057
8	33.475(163)			0.053	0.046
9	33.659(148)			0.050	0.028
10	33.791(133)			−0.020	−0.008
11	33.888(118)			−0.019	−0.020
12	33.960(101)			−0.018	−0.045
13	34.021(84)			−0.018	−0.100
14	34.084(71)			−0.018	−0.142
15	34.100(60)			−0.017	−0.181
16	34.118(48)			−0.017	−0.249
17	34.152(39)			−0.017	−0.334
18	34.177(33)			−0.017	
19	34.196(22)			−0.019	
20	34.208(11)			−0.019	
⋮					
∞[a]	34.311				

[a]NIST atomic database [18]. $\lvert\Delta E\rvert$: energy differences relative to the experimental data.

Table 4. Energy resonances (E) and quantum defect (δ) of the $2D^0 2s^2 2p^2(^1D)ns\ (^2D)$ Rydberg series observed in the photoionization spectra originating from the $2D^0$ metastable states of O^+. The present results (MAOT) are compared to the Advanced Light Source (ALS) of Aguilar *et al.* [2]. The results are expressed in eV. The energy uncertainties in the present calculations are indicated into parenthesis.

	$E(eV)$			δ	
n	MAOT	ALS	$\lvert\Delta E\rvert$	MAOT	ALS
6	32.267(200)	32.267	0.000	0.836	0.836
7	32.881(200)	32.881	0.000	0.825	0.825
8	33.247(165)	33.251	0.004	0.824	0.825
9	33.496(151)	33.498	0.002	0.824	0.804
10	33.678(130)			0.824	
11	33.810(91)			0.824	
10	33.908(62)			0.823	
11	33.976(43)			0.823	
12	34.040(36)			0.823	
13	34.099(28)			0.823	
14	34.131(21)			0.823	
15	34.163(17)			0.824	
16	34.175(14)			0.824	
17	34.182(9)			0.824	
18	34.197(7)			0.824	
19	34.217(5)			0.824	
20	34.231(2)			0.824	
⋮					
∞[a]	34.311				

[a]NIST atomic database [18]. $\lvert\Delta E\rvert$: energy differences relative to the experimental data.

eV; $\sigma_1 = 6.067877676 \pm 0.430724379$ *and* $\sigma_2 = -2.360746016 \pm 0.19010132$. Comparison shows that the maximum energy deviation is at 0.004 up to n =9. This indicates the very good accuracy between the results. For $n \geq 10$ it should be underlined that, since the *MAOT* formalism reproduces excellently the experimental measurements [2], the present results quoted in **Table 4** for the $2D^0 2s^2 2p^2(^1D)ns\ (^2D)$ levels may be a very good representative of the nonexistent experimental data.

In **Table 5**, we compare the present *MAOT* energy resonances (E) and quantum defect (δ) of the $2D^0 2s^2 2p^3(^3D)np(^2P)$ Rydberg series relatively to the $2D^0$_ metastable state of O^+ ion to experimental data [2]. Our current energy positions are calculated from Equations (11) with $Z = 8$ along with $m = 3$, and $q = 4$, E_∞ = 46.707 eV, $\sigma_1 = 6.100874328 \pm 0.092439223$ *and* $\sigma_2 = -1.664259453 \pm 0.207487744$. We note the present quantum defect is almost constant and positive along the series with the effective charge $Z^* \geq Z_{core}$. Thus up to $n = 9$, the agreements are seen to be very good with the maximum energy difference relative to the experimental data is at 0.004 eV.

Table 5. Energy resonances (E) and quantum defect (δ) of the $2D^0 2s^2 2p^3(^3D)np(^2P)$ Rydberg series observed in the photoionization spectra originating from the $2D^0$ metastable states of O^+. The present results (MAOT) are compared to the Advanced Light Source (ALS) of Aguilar *et al.* [2]. The results are expressed in eV. The energy uncertainties in the present calculations are indicated into parenthesis.

	$E(eV)$			δ	
n	MAOT	ALS	$\lvert\Delta E\rvert$	MAOT	ALS
3	37.604(200)	37.604	0.000	0.551	0.551
4	42.149(200)	42.149	0.000	0.534	0.534
5	43.981(146)	43.977	0.004	0.520	0.511
6	44.886(102)	44.882	0.004	0.520	0.496
7	45.405(73)	45.402	0.003	0.520	0.470
8	45.660(61)	45.658	0.002	0.520	0.696
9	45.944(49)	45.943	0.001	0.519	0.397
10	46.085(42)			0.519	
11	46.178(28)			0.519	
12	46.250(20)			0.518	
13	46.311(17)			0.518	
14	46.378(12)			0.518	
15	46.422(10)			0.518	
16	46.460(9)			0.517	
17	46.496(8)			0.519	
18	46.521(7)			0.519	
19	46.544(6)			0.519	
20	46.565(5)			0.519	
⋮					
∞[a]	46.707				

[a]NIST atomic database [18]. $\lvert\Delta E\rvert$: energy differences relative to the experimental data.

In **Table 6**, we compare the present *MAOT* energy resonances (E) and quantum defect (δ) of the $2D^0 2s^2 2p^3(^3D^0)np(^2F)$ Rydberg series relatively to the $2D^0$_ metastable state of O^+ ion to experimental data [2]. All our energy values are obtained empirically using Equation (12) and converted into (eV) for direct comparison. In a few series where discrepancies are observed, the maximum energy difference relative to the experimental data is at 0.003 eV. The agreements are seen to be very good and this may expect our results for $n > 6$ to be accurate.

In **Table 7**, we quote the present *MAOT* results for energy resonances (E) and quantum defect (δ) of the $4S^0 2s^2 2p^3(^5S^0)np(^4P)$ Rydberg series relatively to the $4S^0$_metastable state of O^+ ion. The current energy positions are calculated from Equations (13) along with $Z = 8$, $m = 4$, *and* $q = 5$, $\sigma_1 = 5.99920618 \pm 0.207827476$ and $\sigma_2 = -1.0645904 \pm 0.429419911$. All these screening constant are evaluated using the Advaced Light Source (ALS) experimental results of Aguilar *et al.* [2], and take from NIST [18] the E_∞ energy limits which is 42.586 eV. Then our results

Table 6. Energy resonances (E) and quantum defect (δ) of the $2D^0 2s^2 2p^3(^3D^0)np(^2F)$ Rydberg series observed in the photoionization spectra originating from the $2D^0$ metastable states of O^+. The present results (*MAOT*) are compared to the Advanced Light Source (ALS) of Aguilar *et al.* [2]. The results are expressed in eV. The energy uncertainties in the present calculations are indicated into parenthesis.

	$E(eV)$			δ	
n	*MAOT*	*ALS*	$\lvert\Delta E\rvert$	*MAOT*	*ALS*
3	38.686(200)	38.686	0.000	0.391	0.391
4	42.409(200)	42.409	0.000	0.430	0.430
5	44.075(174)	44.072	0.003	0.429	0.430
6	44.920(140)	44.919	0.001	0.429	0.438
7	45.101(111)			0.428	
8	45.511(76)			0.428	
9	45.825(65)			0.428	
10	46.000(49)			0.428	
11	46.117(37)			0.427	
12	46.241(25)			0.427	
13	46.300(20)			0.427	
14	46.338(18)			0.426	
15	46.392(13)			0.426	
16	46.430(8)			0.426	
17	46.466(6)			0.428	
18	46.500(5)			0.428	
19	46.528(4)			0.428	
20	46.551(2)			0.428	
⋮					
∞[a]	46.620				

[a]NIST atomic database [18]. $\lvert\Delta E\rvert$: energy differences relative to the experimental data.

Table 7. Energy resonances (E) and quantum defect (δ) of the $4S^0 2s^2 2p^3(^5S^0)np(^4P)$ Rydberg series observed in the photoionization spectra originating from the $4S^0$ metastable states of O^+. The present results (*MAOT*) are compared to the Advanced Light Source (ALS) of Aguilar *et al.* [2]. The results are expressed in eV. The energy uncertainties in the present calculations are indicated into parenthesis.

	$E(eV)$			δ	
n	*MAOT*	*ALS*	$\lvert\Delta E\rvert$	*MAOT*	*ALS*
4	38.216(200)	38.216	0.000	0.477	0.477
5	39.919(200)	39.919	0.000	0.495	0.495
6	40.776(190)	40.773	0.003	0.540	0.543
7	41.209(168)	41.206	0.003	0.539	0.753
8	41.676(147)	41.674	0.002	0.538	0.336
9	41.879(122)	41.878	0.001	0.538	0.321

Continued

10	42.022(110)	42.021	0.001	0.537	0.309
11	42.122(99)	42.121	0.001	0.537	0.346
12	42.168(81)	42.167	0.001	0.537	0.795
13	42.196(66)			0.536	
14	42.225(53)			0.536	
15	42.251(40)			0.536	
16	42.273(29)			0.538	
17	42.294(21)			0.538	
18	42.317(17)			0.538	
19	42.329(14)			0.538	
20	42.340(12)			0.537	
⋮					
∞[a]	42.586				

[a]NIST atomic database [18]. $|\Delta E|$: energy differences relative to the experimental data.

are converted into eV for direct comparison by using the infinite Rydberg (1 Ry = 0.5 a.u = 13.605698 eV). It is seen that the data obtained compared very well to the experimental data of Aguilar *et al.* [2]. Up to $n = 12$, the maximum energy differences relative to the experimental data is less than 0.004 eV. For $n = 12$, our *MAOT* value at 42.168 eV agrees well with the experimental data of Aguilar at 42.167 eV. This may expect our results *for* $n > 12$ to be accurate.

This indicates the excellent agreements between the present calculations and the experimental measurements for energy positions.

4. Summary and Conclusion

In this paper, energy resonances of the $2D^0\_2s^22p^2(^1D)nd(^2F)$; $2D^0\_2s^22p^2(^1D)nd(^2D)$; $2D^0\_2s^22p^2(^1D)nd(^2P)$; $2D^0\_2s^22p^2(^1D)ns(^2D)$; $2D^0\_2s^22p^3(^3D)np(^2P)$; $2D^0\_2s^22p^3(^3D^0)np(^2F)$, *and* $4S^0\_2s^22p^3(^5S^0)np(^4P)$ Rydberg series in the photoionization spectra originating from $2D^0$ and $4S^0$ metastable state of O^+ ions are reported using the Modified Orbital Atomic Theory (*MAOT*). It has been demonstrated the simplicity of the *MAOT* semi-empirical procedure to calculate accurate values energies without having to resort to either a complex mathematical formalism nor to a specific calculation code via a tedious computer program. This work may be of interest for future experimental and theoretical studies in the photoabsorption spectrum of O^+. The simplicity of the presented procedure, allows to obtain very accurate values of the resonance energies up to highly excited Rydberg states ($n \geq 20$).

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Conflicts of Interest

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

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