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Photoionization Study of the $2s^22p^2(^1D)ns(^2D)$, $2s^22p^2(^1D)nd(^2P)$, $2s^22p^2(^1D)nd(^2S)$, $2s^22p^2(^1S)nd^2D$, and $2s^22p^3(^3P)np(^2D)$ Rydberg Series of O+ Ions via the Modified Atomic Orbital Theory

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Abstract

We report in this paper energy positions of the $2P^\circ\_2s^22p^2(^1D)nd\ ^2P$, $2P^\circ\_2s^22p^2(^1D)nd\ ^2S$, $2P^\circ\_2s^22p^2(^1D)ns\ ^2D$, $2P^\circ\_2s^22p^2(^1S)nd\ ^2D$, and $2P^\circ\_2s^22p^3(^3P)np\ ^2D$ Rydberg series in the photoionization spectra originating from 2P° metastable state of O+ ions. Calculations are performed up to n = 30 using the Modified Orbital Atomic Theory (MAOT). The present results are compared to the experimental data of Aguilar 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

The important role of studying Photoionization is a fundamental processes playing in laboratory and astrophysical systems such as nebulae plasmas [1], in inertial-confinement fusion experiments [2] and contributing to plasma opacity and radiation transfer inside plasmas. Thus, quantitative measurements of photoionization of ions provide precision data on ionic structure, and guidance to the development of theoretical approaches of multielectron interactions. Greatest attention has been concentrated on studying Rydberg series of O+ ions for which photoabsorption from low-lying metastable states of open-shell ions has been shown to be important in the earth's upper atmosphere as well as in astrophysical plasmas. Formerly, studies on the O+ ion have been focused on ionization using the merged-beam technique. Thus, Aguilar *et al.* [3] performed the first experiment on the Absolute photoionization of O+ from 29.7 to 46.2 eV above the first ionization threshold, using a merged-beam line at the Advanced Light Source (ALS).

Therefore, it is an imperative task for physicists to provide accurate photoionization data for the modeling of astrophysical and laboratory plasmas.

The Opacity Project atomic database (at the Astronomic DataCenter of Strasbourg, France) was formed to re-estimate stellar envelope opacities in terms of atomic data computed by *ab initio* methods [4]. All these efforts led to the creation of several atomic databases widely used for astrophysical calculations [3].

In the present paper, we intend to provide accurate data on the photoionization of O+ ions 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 of SOW *et al.* [5] [6] [7] [8] to reproduce excellently experimental data from merged beam facilities. For this purpose, we report calculations of energy resonances for the $2P^{\circ}\_2s^{2}2p^{2}(^{1}D)nd\ ^{2}P$, $2P^{\circ}\_2s^{2}2p^{2}(^{1}D)nd\ ^{2}S$, $2P^{\circ}\_2s^{2}2p^{2}(^{1}D)ns\ ^{2}D$ $2P^{\circ}\_2s^{2}2p^{2}(^{1}S)nd\ ^{2}D$, and $2P^{\circ}\_2s^{2}2p^{3}(^{3}P)np\ ^{2}D$ Rydberg series of O+ ions up to $n = 30$, via the MAOT procedure along with the quantum defect theory.

Energy resonances and quantum-defect are compared to the only available experimental data of ALS [3].

Section 2 gives MAOT theory with a brief description of the formalism and the analytical expressions used in the calculations. In Section 3, we present and discuss the results obtained, compared to available experimental. 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 ($\nu\ell$)-given orbital is expressed in the form [8] [9].

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

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

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

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 this formula (2), L characterizes the considered quantum state (S, P, D …) and the symbol π is the parity of the system.

In the photoionisation study, energy resonances are generally measured relatively to the E∞ 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 [10] (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 $\sigma_i({}^{2S+1}L_J)$-screening 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 values along all the considered series. The value of μ is fixed to 1 and 2 during the iteration. The quantum defect 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.

2.2. Energy Resonances of the $2P^\circ\_2s^22p^2({}^1D)nd({}^2P)$; $2P^\circ\_2s^22p^2$ $({}^1D)nd({}^2S)$; $2P^\circ\_2s^22p^2$ $({}^1D)$ ns $({}^2D)$; $2P^\circ\_2s^22p^2$ $(1S)nd(2D)$ and $2P^\circ\_2s^22p^3({}^3P)np({}^2D)$ Rydberg Series from $2P^\circ$ Metastable State of O+

In the framework of the MAOT formalism, the energy positions of the $2P^\circ\_2s^22p^2({}^1D)nd({}^2P)$; $2P^\circ\_2s^22p^2$ $({}^1D)nd({}^2S)$; $2P^\circ\_2s^22p^2$ $({}^1D)$ ns $({}^2D)$; $2P^\circ\_2s^22p^2$ $(1S)nd(2D)$ and $2P^\circ\_2s^22p^3({}^3P)np({}^2D)$ prominent Rydberg series from 2P° metastable state of O+ are given by (in Rydberg units)

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

$$E_n = E_\infty - \frac{1}{n^2}\left\{Z - \sigma_1 - \frac{\sigma_2}{n} + \sigma_2 \times (n-m) \times (n-q) \times \left[\frac{1}{(n+q-s)^3} + \frac{1}{(n+m-s)^3} + \frac{1}{(n+m+s)^3} + \frac{1}{(n+m-s)^4} + \frac{1}{(n+q-m+s)^5}\right]\right\}^2 \quad (6)$$

Using the experimental data of ALS [3], we obtain (in eV) $E_5 = 30.393 \pm 0.15$ ($m = 5$) and $E_6 = 31.081 \pm 0.15$ ($q = 6$) respectively for the $2P^{\circ}\_2s^22p^2(^1D)5d\,^2P$ and $2P^{\circ}\_2s^22p^2(^1D)6d\,^2P$ levels. From NIST [11], we find $E_\infty = 32.617$ eV. Using these data, Equation (6) gives $\sigma_1 = 6.012 \pm 0.251$ and $\sigma_2 = -0.166 \pm 0.009$

- **For 2P°_2s²2p² (¹D)nd(²S) levels:**

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

For the $2P^{\circ}\_2s^22p^2(^1D)5d\ ^2S$ and $2P^{\circ}\_2s^22p^2(^1D)6d\ ^2S$ levels, we find using the experimental data of ALS *et al.* [3], $E_5 = 30.213 \pm 0.150$ ($m = 5$) and $E_6 = 30.905 \pm 0.150$ ($q = 6$). From NIST [11], we find $E_\infty = 32.617$ eV Equation (7) provides then $\sigma_1 = 6.061 \pm 0.185$ and $\sigma_2 = -0.367 \pm 0.092$

- **For 2P°_2s²2p² (¹D) ns (²D) levels**

$$E_n = E_\infty - \frac{1}{n^2}\left\{Z - \sigma_1 - \frac{\sigma_2}{n} + \sigma_2 \times (n-m) \times (n-q) \times \left[\frac{1}{(n+q-s)^3} + \frac{1}{(n+q+s-m)^4} + \frac{1}{(n+q-s)^4} + \frac{1}{(n+m-s)^4} + \frac{1}{(n+q-m+3s)^5}\right]\right\}^2 \quad (8)$$

For the $2P^{\circ}\_2s^22p^2$ (^1D) $6s$ (^2D) and $2P^{\circ}\_2s^22p^2$ (^1D) $7s$ (^2D) levels the experimental energy positions ALS *et al.* [3] are, $E_6 = 30.578 \pm 0.15$ ($m = 6$) and $E_7 = 31.188 \pm 0.15$ ($q = 7$). From NIST [11], we find $E_\infty = 32.617$ eV. In that case, we find using Equation (8) $\sigma_1 = 6.056 \pm 0.322$ and $\sigma_2 = -2.274 \pm 0.413$

- **For 2P°_2s²2p² (1S)nd(²D) levels**

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

From ALS of Aguilar *et al.* [3], we obtain for the $2P^{\circ}\_2s^22p^2$ $(1S)4d(2D)$ and $2P^{\circ}\_2s^22p^2$ $(1S)5d(^2D)$ $E_4 = 31.924 \pm 0.15$ ($m = 4$) and $E_5 = 33.217 \pm 0.15$ ($q = 5$). From NIST [11], we find $E_\infty = 35.458$ eV. We find then using Equation (9) $\sigma_1 = 6.008 \pm 0.167$ and $\sigma_2 = -0.187 \pm 0.05$.

- **For 2s²2p³(³P)np(²D) levels**

$$E_n = E_\infty - \frac{1}{n^2}\left\{Z - \sigma_1 - \frac{\sigma_2}{n} + \sigma_2 \times (n-m) \times (n-q) \times \left[\frac{1}{(n-s)^2} + \frac{1}{(n+s-m)^2} - \frac{1}{(n+s-m)^3} + \frac{1}{(n+s-m)^4}\right]\right\}^2 \quad (10)$$

From ALS *et al.* [3], we obtain for the $2P^{\circ}\_2s^{2}2p^{3}(^{3}P)3p(^{2}D)$ *and* $2P^{\circ}\_2s^{2}2p^{3}(^{3}P)4p(^{2}D)$ $E_3 = 39.478 \pm 0.15$ ($m = 3$) and $E_4 = 43.115 \pm 0.15$ ($q = 4$). From NIST [11], we find $E_\infty = 47.527$eV. We find then using Equation (10) $\sigma_1 = 5.411 \pm 0.411$ and $\sigma_2 = -0.844 \pm 0.022$

3. Results and Discussions

The results obtained in the present paper are listed in **Tables 1-5** and compared with the Advanced Light Source experimental data of Aguilar *et al.* [3].

In **Table 1**, we quote the present MAOT results for energy resonances (E) and quantum defect (δ) of the $2P^{\circ}\_2s^{2}2p^{2}(^{1}D)nd(^{2}P)$ Rydberg series relatively to the 2P°_metastable state of O+ ion. The current energy positions are calculated from equations (6) along with $Z = 8$, $m = 5$, and $q = 6$, $\sigma_1 = 6.012 \pm 0.251$ and $\sigma_2 = -0.166 \pm 0.009$. All these screening constant are evaluated using the Advanced Light Source (ALS) experimental results of Aguilar *et al.* [3], and take from NIST [11] the E_∞ energy limits which is 32.617 eV. Then our results 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.* [3].

Up to $n = 11$, the maximum energy differences relative to the experimental data is less than 0.006 eV. In addition, the present quantum defect is almost constant up to $n = 30$. This may expect our results for $n > 11$ to be accurate.

In **Table 2**, we compare the present MAOT energy resonances (E) and quantum defect (δ) of the $2P^{\circ}\_2s^{2}2p^{2}(^{1}D)nd(^{2}S)$ Rydberg series relatively to the 2P°_metastable state of O+ ion to experimental data [3]. All our energy values are obtained empirically using Equation (7) and converted into (eV) for direct comparison. Here again, the agreements are seen to be very good. Along the series, the present quantum defect is almost constant.

In **Table 3**, we show a comparison of the energy resonances (E) and quantum defect (δ) of the $2P^{\circ}\_2s^{2}2p^{2}(^{1}D)ns$ (^{2}D) Rydberg states relatively to the 2P°_metastable state of O+ ion. The current energy positions are calculated from equations (8) along with $Z = 8$, $m = 6$, and $q = 7$, $\sigma_1 = 6.056 \pm 0.322$ and $\sigma_2 = -2.274 \pm 0.413$. The agreements between the studies are seen to be very good and the quantum defect is almost constant along the series. The agreements between the MOAT results and experimental data are seen to be very good. Along all the series investigated, the quantum defect is practically constant. This may expect our results up to $n = 30$ to be accurate.

In **Table 4**, we list the present energy resonances (E) and quantum defect (δ) for the 2P°$\_2s^{2}2p^{2}(^{1}S)nd$ (^{2}D) Rydberg states relatively to the 2P°_metastable state of O+ ion compared to the experimental data [3]. The current energy positions are calculated from equations (9) along with $Z = 8$, $m = 4$, and $q = 5$, $E_\infty = 35.458$ eV; $\sigma_1 = 6.008 \pm 0.167$ and $\sigma_2 = -0.187 \pm 0.05$. Comparison shows that the maximum energy deviation is at 0.006 up to $n = 14$. This indicates the very good accuracy between the results. For $n \geq 15$ it should be underlined that, since the MAOT formalism reproduces excellently the experimental measurements [3], the present results quoted in **Table 4** for the $2P^o\_2s^22p^2(^1S)nd\,(^2D)$ levels may be a very good representative of the nonexistent experimental data.

Table 1. Energy resonances (E) and quantum defect (δ) of the $2P^o\_2s^22p^2\,(^1D)nd\,(^2P)$ Rydberg series observed in the photoionization spectra originating from the $2P^o$ 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 and in the experimental data are indicated into parenthesis.

	$E\,(eV)$			δ	
n	MAOT	ALS	$\lvert\Delta E\rvert$	MAOT	ALS
5	30.393 (150)	30.393 (150)	0.000	0.054	0.054
6	31.081 (150)	31.081 (150)	0.000	0.048	0.048
7	31.496 (148)	31.496 (150)	0.000	0.032	0.033
8	31.763 (138)	31.762 (150)	0.001	0.018	0.023
9	31.955 (122)	31.948 (150)	0.005	0.004	−0.015
10	32.074 (106)	-----	---------	−0.008	− 0.092
11	32.170 (92)	32.169 (150)	0.001	−0.020	−0.018
12	32.241 (81)			−0.031	
13	32.297 (71)			−0.032	
14	32.341 (63)			−0.033	
15	32.377 (56)			−0.034	
16	32.406 (50)			−0.035	
17	32.431 (45)			−0.036	
18	32.451 (41)			−0.036	
19	32.468 (37)			−0.037	
20	32.483 (34)			−0.037	
21	32.495 (31)			−0.037	
22	32.506 (28)			−0.038	
23	32.515 (26)			−0.038	
24	32.524 (24)			−0.038	
25	32.531 (22)			−0.039	
26	32.538 (21)			−0.039	
27	32.543 (19)			−0.039	
28	32.549 (18)			−0039	
29	32.553 (17)			−0.038	
30	32.557 (16)			−0.039	
…					
∞^a	32,617				

[a] NIST atomic database [11]. $\lvert\Delta E\rvert$: energy differences relative to the experimental data.

Table 2. Energy resonances (E) and quantum defect (δ) of the $2P^{\circ}\_2s^22p^2\ (^1D)nd\ (^2S)$ Rydberg series observed in the photoionization spectra originating from the $2P^{\circ}$ 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 and in the experimental data are indicated into parenthesis.

n	$E\,(eV)$			°	
	MAOT	ALS	$\lvert\Delta E\rvert$	MAOT	ALS
5	30.413 (200)	30.413 (150)	0.000	0.031	0.031
6	31.105 (200)	31.105 (150)	0.000	0.001	0.001
7	31.517 (182)	--------		0.034	0.033
8	31.781 (161)	--------		0.020	0.023
9	31.961 (140)	--------		−0.016	−0.017
10	32.088 (122)	--------		−0.103	−0.092
11	32.182 (106)	--------		−0.018	−0.018
12	32.252 (93)			−0.026	
13	32.307 (82)			−0.023	
14	32.350 (73)			−0.029	
15	32.385 (65)			−0.022	
16	32.414 (58)			−0.022	
17	32.437 (52)			−0.027	
18	32.457 (47)			−0.023	
19	32.473 (43)			−0.028	
20	32.488 (39)			−0.024	
21	32.500 (36)			−0.029	
22	32.510 (33)			−0.024	
23	32.519 (30)			−0.028	
24	32.527 (28)			−0.023	
25	32/534 (26)			−0.027	
26	32.541 (24)			−0.021	
27	32.546 (23)			−0.025	
28	32.551 (21)			−0.029	
29	32.556 (20)			−0.023	
30	32.560 (19)			−0.027	
…					
∞^a	32,617				

^{a}NIST atomic database [11]. $\lvert\Delta E\rvert$: energy differences relative to the experimental data.

Table 3. Energy resonances (E) and quantum defect (δ) of the $2P^o\_2s^22p^2\ (^1D)ns\ (^2D)$ Rydberg series observed in the photoionization spectra originating from the $2P^o$ 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 and in the experimental data are indicated into parenthesis.

n	$E\,(eV)$			°	
	MAOT	ALS	$\lvert\Delta E\rvert$	MAOT	ALS
6	30.578 (150)	30.578 (150)	0.000	0.834	0.834
7	31.188 (150)	31.188 (150)	0.000	0.829	0.829
8	31.562 (135)	31.561 (150)	0.002	0.826	0.822
9	31.803 (119)			0.824	
10	31.971 (104)			0.822	
11	32.092 (93)			0.820	
12	32.182 (79)			0.818	
13	32.250 (70)			0.817	
14	32.304 (62)			0.815	
15	32.347 (55)			0.814	
16	32.381 (49)			0.813	
17	32.409 (44)			0.811	
18	32.433 (40)			0.810	
19	32.453 (36)			0.809	
20	32.469 (33)			0.808	
21	32.484 (30)			0.807	
22	32.496 (29)			0.805	
23	32.507 (26)			0.804	
24	32.516 (24)			0.803	
25	32.524 (22)			0.802	
26	32.531 (20)			0.801	
27	32.538 (19)			0.800	
28	32.543 (18)			0.799	
29	32.549 (17)			0.799	
30	32.553 (16)			0.800	
…					
∞^a	32,617				

^{a}NIST atomic database [11]. $\lvert\Delta E\rvert$: energy differences relative to the experimental data.

Table 4. Energy resonances (E) and quantum defect (δ) of the $2P^{\circ}\_2s^{2}2p^{2}\ (^{1}S)nd\ (^{2}D)$ Rydberg series observed in the photoionization spectra originating from the $2P^{\circ}$ 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 and in the experimental data are indicated into parenthesis.

n	$E\,(eV)$			°	
	MAOT	ALS	$\|\Delta E\|$	MAOT	ALS
4	31.924 (150)	31.924 (150)	0.000	0.076	0.076
5	33.217 (150)	33.217 (150)	0.000	0.072	0.072
6	33.911 (125)	33.910 (150)	0.001	0.072	0.071
7	34.332 (103)	34.328 (150)	0.004	0.071	0.061
8	34.599 (85)	34.597 (150)	0,002	0.071	0.050
9	34.785 (70)	34.782 (150)	0.003	0.071	0.028
10	34.912 (59)	34.909 (150)	0.003	0.070	0.044
11	35.012 (51)	35.008 (150)	0.004	0.070	0.004
12	35.088 (44)	35.082 (150)	0.006	0.069	−0.030
13	35.147 (38)	35.145 (150)	0.002	0.069	−0.185
14	35.185 (33)	35.183 (150)	0.002	0.068	−0.066
15	35.222 (29)	35.219 (150)	0.003	0.068	−0.088
16	35.244 (26)			0.067	
17	35.268 (23)			0.067	
18	35.289 (21)			0.066	
19	35.306 (19)			0.066	
20	35.321 (17)			0.066	
21	35.334 (16)			0.067	
22	35.345 (14)			0.067	
23	35.355 (13)			0.067	
24	35.363 (12)			0.067	
25	35.370 (11)			0.067	
26	35.377 (11)			0.067	
27	35.383 (10)			0.067	
28	35.388 (09)			0.067	
29	35.393 (09)			0.067	
30	35.397 (08)			0.067	
…					
∞[a]	35,458				

[a]NIST atomic database [11]. $|\Delta E|$: energy differences relative to the experimental data.

Table 5. Energy resonances (E) and quantum defect (δ) of the $2P^o\_2s^22p^3\ (3P^o)nd\ (^2D)$ Rydberg series observed in the photoionization spectra originating from the $2P^o$ 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 and in the experimental data are indicated into parenthesis.

n	$E(eV)$			°	
	MAOT	ALS	$\lvert\Delta E\rvert$	MAOT	ALS
3	39.478 (150)	39.478 (150)	0.000	0.436	0.436
4	43.115 (150)	43.115 (150)	0.000	0.576	0.576
5	45.092 (150)	45.093 (150)	0.001	0.485	0.480
6	46.009 (145)			0.483	
7	46.499 (138)			0.483	
8	46.788 (135)			0.483	
9	46.971 (133)			0.483	
10	47.095 (132)			0.482	
11	47.181 (131)			0.479	
12	47.244 (124)			0.479	
13	47.292 (116)			0.479	
14	47.328 (110)			0.480	
15	47.357 (106)			0.480	
16	47.380 (94)			0.480	
17	47.398 (84)			0.480	
18	47.412 (75)			0.480	
19	47.425 (68)			0.481	
20	47.436 (62)			0.481	
21	47.445 (56)			0.481	
22	47.453 (52)			0.481	
23	47.460 (47)			0.481	
24	47.466 (44)			0.481	
25	47.471 (40)			0.481	
26	47.475 (37)			0.481	
27	47.479 (35)			0.480	
28	47.483 (32)			0.480	
29	47.486 (30)			0.480	
30	47.489 (28)			0.480	
…					
∞^a	47,527				

[a] NIST atomic database [11]. $\lvert\Delta E\rvert$: energy differences relative to the experimental data.

In Table 5, we compare the present MAOT energy resonances (E) and quantum defect (δ) of the $2P^{\circ}\_2s^2 2p^2(^1D)nd(^2S)$ Rydberg series relatively to the 2P°_metastable state of O+ ion to experimental data [3]. Our current energy positions are calculated from Equations (10) with $Z = 8$ along with $m = 3$, and $q = 4$, $E_{\infty} = 47.527\ eV$, $\sigma_1 = 5.411 \pm 0.411$ and $\sigma_2 = -0.844 \pm 0.022$. Here again, the agreements are seen to be very good. Along the series, the present quantum defect is almost constant. In a few series where discrepancies are observed, the maximum energy difference relative to the experimental data is at 0.001 eV. This indicates the excellent agreements between the present calculations and the experimental measurements for energy positions.

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.

4. Summary and Conclusion

In this paper, energy resonances of the $2s^2 2p^2(^1D)ns(^2D)$, $2s^2 2p^2(^1D)nd(^2P)$, $2s^2 2p^2(^1D)nd(^2S)$, $2s^2 2p^2(^1S)nd\ (^2D)$, and $2s^2 2p^3(^3P)np\ (^2D)$ Rydberg series in the photoionization spectra originating from 2P metastable state of O+ ions are reported in this paper using the Modified Orbital Atomic Theory (MAOT). Over the entire Rydberg series investigated, it is shown that the present MOAT results agree very well with the only available experimental data of ALS [3]. A host of accurate data up to $n = 30$ are quoted in the recent work. The very good result obtained is this work points out the possibilities to use the MAOT 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 O^+.

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Conflicts of Interest

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

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