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Photoionization Study of Cl II, Ar II and Kr II Ions Using the Modified Atomic Orbital Theory

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Abstract

Resonance energies of the Cl II-[$3s^23p^3(^2D_{5/2})$]*n*d and [$3s^23p^3(^2P_{3/2})$]*n*d, Ar II-$3s^23p^4(^1D_2)$*n*s, *n*d and of the Kr II [$4s^24p^4(^1D_2)$]*n*s, *n*d and $4s^24p^4(^3P_2,^3P_1)$]*n*s, $4s^24p^4(^3D_2)$]*n*s, *n*d and $4s^24p^4(^3D_2$, $^1S_0)$]*n*s, *n*d Rydberg series are reported. Natural widths of the Ar II-[$3s^23p^4(^1D_2)$]*n*s, *n*d series are also reported. Calculations are done in the framework of the Modified Atomic Orbital Theory (MAOT). Excellent agreements are obtained with available theoretical and experimental data. High lying accurate resonance energies up to $n = 40$ are tabulated. The possibility to use the MAOT formalism report rapidly with an excellent accuracy the position of the excitation resonances as well as their width within simple analytical formulae is demonstrated.

Keywords

Resonance Energies, Rydberg Series, Natural Widths, Modified Atomic Orbital Theory (MAOT)

1. Introduction

In many astrophysical systems such as stars and nebulae, the main process governing light-atomic species interaction is Photoionization. Of great important ions interesting to investigate are Cl II (Cl^+), Ar II (Ar^+) and Kr II (Kr^+) ions. As far as Cl II is concerned, its interest is connected with it abundance in photoionized astrophysical objects. In the past, various studies have indicated the great importance of Cl II ions abundances for understanding extragalactic HII regions [1]. In addition, emission lines of Cl II ions have been observed in the spectra of the Io torus [2] and in the optical spectra of planetary nebulae NGC 6741 and IC 5117 [3]. In a very recent past, Hernández *et al.*, [4] measured at the Advanced Light Source at Lawrence Berkeley National Laboratory absolute photoionization cross-sections for the of Cl II ions using the merged beams photon-ion technique at a photon energy resolution of 15 meV in the energy range 19 - 28 eV. Using the Dirac-Coulomb *R*-matrix (DCR) method, McLaughlin, [5] performed calculations in the same photon energy range that in the ALS experiments [4] to assign and identify the resonance series in the ALS spectra of the Cl II ions. In these experimental works, the $3s^23p^3nd$ states have been identified in the Cl II spectra as the prominent Rydberg series belonging to the $3p \to nd$ transitions. The weaker $3s^23p^3ns$ Rydberg series, identified as $3p \to ns$ transitions and window resonances $3s3p^4(^4P)$ np features, due to $3s \to np$ transitions, have also been found in the spectra [5]. Besides, one of the important elements to study is Argon present in several astrophysical systems. An overabundance of the argon element in the spectra of X-rays of yellow supernovas was revealed by the satellite Chandra [6] dedicated to analyze the stellar object spectra. Furthermore, spectral rays of the argon element were observed in the optical spectra of planetary stars and nebulae [7] [8]. These few examples show the importance of the photoionization study of the argon element from the perspective of astrophysics. In a recent past, Covington *et al.*, [9] performed the first experimental measurements of the photoionization cross-section of the Ar II ion. These authors also determined the resonance energies and natural widths related to the dominant Rydberg series $3s^23p^4(^1D_2)ns$, nd and $3s^23p^4(^1S_0)ns$, nd in the emission spectra of the Ar II ions. These energies were relatively measured at the metastable state Ar II $(^2P°_{1/2})$ and at the ground state Ar II $(^2P°_{3/2})$. As far as Krypton is concerned, it is also an element of major importance for diagnosing stellar plasmas such as stars and planetary nebulae as well as for diagnosing laboratory plasmas such as those obtained by inertial fusion. In a recent past, Hinojosa *et al.*, [10] experimentally studied the photoionization of the Kr II ion at ALS at Berkley in the photonic energy range of 23 - 39 eV. In the photoionization spectra, these authors observed several Rydberg series, including the Kr II $[4s^24p^4(^1D_2)]$ ns, nd series converging toward the excitation threshold Kr II $[4s^24p^4(^1D_2)]$. Very recently, Sakho, [11] applied the Screening constant by unit nuclear charge (SCUNC) formalism to report precise data belonging to various Rydberg series of Ar II and Kr II as observed in the works of Covington *et al.*, [9] for Ar II and of Hinojosa *et al.*, [10] for Kr II. In the present study, we use the Modified atomic orbital theory [12] [13] [14] [15] [16] to report accurate high lying resonance energies of the Cl I-$[3s^23p^3(^2D_{5/2})]nd$ and $[3s^23p^3(^2P_{3/2})]nd$, Ar II-$3s^23p^4(^1D_2)ns$, nd and of the Kr II $[4s^24p^4(^1D_2)]ns$, nd and $4s^24p^4(^3P_2,^3P_1)]ns$, $4s^24p^4(^3D_2)]ns$, nd and $4s^24p^4(^3D_2,\ ^1S_0)]ns$, nd Rydberg series reported. Natural widths of the Ar II-$[3s^23p^4(^1D_2)]$ ns, nd series are also reported. In Section 2, a brief description of the MAOT formalism is given. The results are present in Section 3. Section 4 concludes the study.

2. Theory

2.1. Brief Description of the Modified Atomic Orbital Theory

In the framework of the modified atomic orbital theory (MAOT), the total energy of a (νl)-given orbital is expressed in the form in Rydberg units

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

In Equation (1), σ is the screening constant relative to the electron occupying the (νl)-orbital, l denotes the orbital quantum number, ν stands for the principal quantum number and Z represents the atomic number. In general, the doubly excited states (DES) in two electron systems are labelled as $\left(Nl, nl'\right)^{2S+1}L^{\pi}$. In this notation, N and n denote respectively the principal quantum numbers of the inner and the outer electron, l and l' are their respective orbital quantum numbers, S the total spin, L the total angular momentum and π the parity of the system. For an atomic system of many M electrons, total energy is expressed as follows

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

In the photoionisation study, energy resonances E_n are generally measured relatively to the E_∞ converging limit of a given $({}^{2S+1}L_J)nl$-Rydberg series. For these states [12] [13] [14]

$$\begin{aligned} E_n = E_\infty - \frac{1}{n^2}\Bigg\{ & Z - \sigma_1\left({}^{2S+1}L_J\right) - \sigma_2\left({}^{2S+1}L_J\right) \times \frac{1}{n} \\ & - \sigma_2^{\alpha}\left({}^2P^0_{3/2}, {}^1D_2\right) \times (n-m) \times (n-q) \sum_k \frac{1}{f_k(n,m,q,s)} \Bigg\}^2 \end{aligned} \tag{3}$$

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 $\sigma_i\left({}^{2S+1}L_J\right)$-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 NIST atomic database, 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 α is fixed to 1 and or 2 during the iteration. The quantum defect is calculated from the standard formula

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

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. As far as the natural widths are concerned, they are given by (in Rydberg units)

$$\Gamma_n = \frac{1}{n^2}\Bigg\{Z-\sigma_1'\left({}^{2S+1}L_J\right)-\sigma_2'\left({}^{2S+1}L_J\right)\times\frac{1}{n} -\sigma_2^{\alpha'}\left({}^2P_{3/2}^0,{}^1D_2\right)\times(n-m)\times(n-q)\sum_k\frac{1}{f_k'(n,m,q,s)}\Bigg\}^2 \quad (5)$$

2.2. Expressions of the Resonance Energies and of the Natural Widths

In the present work, for all the Rydberg series investigated for both Cl II, Ar II and Kr II, the resonance energies are given by the formula

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

For the $[3s^23p^4(^1D_2)]ns$ ($j = 1/2$) series originating from the $3s^23p^5\ {}^2P^\circ_{1/2}$ metastable state of Ar II ions, the natural widths are given by (in Rydberg units)

$$\Gamma_n = \frac{1}{n^2}\Bigg\{Z-\sigma_1\left({}^{2S+1}L_J\right)-\sigma_2\left({}^{2S+1}L_J\right)\times\frac{1}{n}+\sigma_2^2\left({}^{2S+1}L_J\right)\times(n-m)\times(n-q) \times\left[\frac{1}{(n+q-m+s+1)^4}+\frac{1}{(n+m+s)^4}+\frac{1}{(n+q+s)^4}+\frac{1}{(n+m-s)^4}\right]\Bigg\}^2 \quad (7)$$

The other expressions for the other series are of type Equation (7).

3. Results and Discussion

The σ_1-screening constants in Equations (6) and (7) are evaluated empirically using the data from Covington *et al.*, [9] Hinojosa *et al.*, [10] and from Hernández *et al.*, [4]. The results obtained as indicated in the caption of the corresponding Table. As far as the σ_2-screening constant is concerned, it is evaluated theoretical from the simple equation $\sigma_2 = Z - Z_{core}$. The electric charge of the core ion is deduced directly from the single Photoionization process for a given X^{p+}-plasma ion

$$h\nu + X^{p+} \to X^{(p+1)} + e^- \Rightarrow Z_{core} = (p+1) \quad (8)$$

So, for Cl II, Ar II and Kr II, we find respectively.

$$h\nu + Cl^+ \to Cl^{2+} + e^-; Z_{core} = 2 \Rightarrow \sigma_2 = 15.00$$

$$h\nu + Ar^+ \to Ar^{2+} + e^-; Z_{core} = 2 \Rightarrow \sigma_2 = 16.00$$

$$h\nu + Kr^+ \to Kr^{2+} + e^-; Z_{core} = 2 \Rightarrow \sigma_2 = 34.00$$

The resonance energies of the $[3s^23p^3(^2D^\circ_{5/2})]nd$ Rydberg series originating from the $3s^23p^4\ {}^3P^\circ_2$ ground state and from the $3s^23p^4\ {}^3P^\circ_1$, $3s^23p^4\ {}^3P^\circ_0$,

$3s^2 3p^4\ ^1S^{\circ}_0$ and $3s^2 3p^4\ ^1D_2$ metastable states of Cl II ions are listed in **Tables 1-8**. Comparisons of the present MAOT calculations are done with the available Dirac-Coulomb *R*-matrix (DCR) calculations [5] and with the ALS experimental data [4]. For both the DCR [5] and ALS [4] studies, the determination of the resonances energies have been limited to $n = 13$ (see **Table 4**). In general due to interaction configuration and other electron-electron effects, the peaks of the cross section overlap involving difficulty for the identification of lines in the atomic spectra with increasing n. But, it can be seen that, the MAOT formulas are enough stable so that very high lying resonances can be tabulate up to $n = 40$ with a quantum defect practically constant along all the series investigated. For many resonances, the uncertain experimental entries in parenthesis are enlightened. In **Table 2**, the resonance energy of the $[3s^2 3p^3 (^2D^{\circ}_{5/2})]11d$ level are equal to 25.493 eV (MAOT), 25.493 eV (DCR) and (25.492 eV) for the ALS uncertain experimental data. The excellent agreement between theories indicate that the ALS data can be stated as accurate at 25.492 eV. The same conclusion can be drawn for the $[3s^2 3p^3 (^2D^{\circ}_{5/2})]8d$ state quoted in **Table 3** where the MAOT prediction at 25.001 eV agree very well with both the DCR value at 24.999 eV [5] and the uncertain ALS measurement [4] equal to (25.000 eV). For this level the ALS data must be considered as precise at 25.000 eV. **Table 4** lists resonance energies of the $[3s^2 3p^3 (^2P^{\circ}_{3/2})]nd$ Rydberg series originating from the $3s^2 3p^4\ ^3P^{\circ}_2$ ground state of the Cl^+ ions. In this table, two uncertain ALS values are quoted for the $[3s^2 3p^3 (^2P^{\circ}_{3/2})]6d$ and $[3s^2 3p^3 (^2P^{\circ}_{3/2})]12d$ levels respectively at (25.745 eV) and (27.114 eV) to be compared to the MAOT predictions at 25.749 eV and 27.113 eV and to the DCR data [5] respectively equal to 25.755 eV and 27.115 eV. For the $n = 11$ and 13, the MAOT calculations respectively at 27.031 eV and 27.176 eV are seen to agree very well with the ALS measurements [4] at 27.031 eV and 27.175 eV. Subsequently the DCR data at 25.755 eV ($n = 6$) and at 27.178 eV ($n = 13$) are probably greater than the accurate data. The ALS experimental entries in parenthesis can be considered as certain at 25.745 eV and 27.114 eV. Besides, the MAOT data at 25.659 eV quoted in **Table 5** is seen to agree very well with the uncertain ALS measurement [4] at (25.660 eV). A slight discrepancy is observed when comparing with the corresponding DCR calculation [5] equal to 25.668 eV. Comparison indicates clearly that the ALS value [4] is correct at 25.660 eV. In **Table 6** and **Table 7**, all the ALS data [4] are certain. In general, good agreements are obtained between theory and experiment. In **Table 8**, the uncertain ALS data [4] at (24.152 eV) for the $[3s^2 3p^3 (^2D^{\circ}_{5/2})]11d$ level is difficult to enlighten. For this level, the MAOT prediction at 24.146 eV compared fairly well with the DCR calculations [5] equal to 24.138 eV. A new measurement or calculation is needed to clarify this uncertain ALS value [4]. Overall, for the entire data quoted in **Tables 2-8**, comparisons indicate that the MAOT formula reproduces with a very good accuracy the ALS measurements [4] via a simple formalism without using computational codes in contrast with the DCR formalism [5]. **Tables 9-11** list resonance energies of the

Table 1. Resonance energies of the $[3s^23p^3(^2D^\circ_{5/2})]nd$ Rydberg series originating from the $3s^23p^4\,^3P^\circ_2$ ground state of the Cl^+ ions converging to the $3s^23p^3(^2D^\circ_{5/2})$ threshold of Cl^{2+}. The present results from the Modified atomic orbital theory (MAOT) are compared with the Dirac-Coulomb *R*-matrix (DCR) calculations of McLaughlin [5] and with the ALS experimental data of Hernández *et al*., [4]. The ALS experimental resonance energies are calibrated to ±0.013 eV. The energy limits is taken from the NIST tabulations of Ralchenko *et al*., [19]. $\sigma_1(^2D_{5/2}) = -0.770 \pm 0.048$; $\sigma_2(^2D_{5/2}) = 15.00$.

n	MAOT	DCR	ALS	MAOT	DCR	ALS
	E	*E*	*E*	δ	δ	δ
6	24.348	24.353	24.348	0.362	0.30	0.38
7	24.824	24.846	24.829	0.363	0.35	0.35
8	25.127	25.130	25.128	0.362	0.30	0.36
9	25.331	25.334	25.335	0.361	0.34	0.34
10	25.474	25.476	25.479	0.360	0.35	0.32
11	25.579	25.584	25.583	0.360	0.30	0.32
12	25.658			0.359		
13	25.719			0.359		
14	25.768			0.358		
15	25.806			0.358		
16	25.838			0.358		
17	25.863			0.358		
18	25.885			0.358		
19	25.903			0.358		
20	25.919			0.358		
21	25.932			0.359		
22	25.944			0.359		
23	25.954			0.359		
24	25.963			0.359		
25	25.970			0.359		
26	25.977			0.360		
27	25.983			0.360		
28	25.989			0.360		
29	25.994			0.361		
30	25.998			0.361		
31	26.002			0.361		
32	26.006			0.361		
33	26.009			0.362		
34	26.012			0.362		
35	26.015			0.362		
36	26.017			0.363		
37	26.019			0.363		
38	26.022			0.363		
39	26.024			0.363		
40	26.025			0.364		
…	…	…	…		…	…
∞	26.060	26.060	26.060			

Table 2. Resonance energies (E) and quantum defect (δ) of the $[3s^2 3p^3(^2D^\circ_{5/2})]nd$ Rydberg series originating from the $3s^2 3p^4\,^3P^\circ_1$ metastable state of the Cl^+ ions converging to the $3s^2 3p^3(^2D^\circ_{5/2})$ threshold of Cl^{2+}. The present results from the Modified atomic orbital theory (MAOT) are compared with the Dirac-Coulomb R-matrix (DCR) calculations of McLaughlin [5] and with the ALS experimental data of Hernández *et al.*, [4]. The ALS experimental resonance energies are calibrated to ±0.013 eV. The energy limits is taken from the NIST tabulations of Ralchenko *et al.*, [19]. $\sigma_1(^2D_{5/2}) = -0.781 \pm 0.048$; $\sigma_2(^2D_{5/2}) = 15.00$.

n	MAOT	DCR	ALS	MAOT	DCR	ALS
	E	E	E	δ	δ	δ
6	24.259	24.264	24.259	0.367	0.36	0.37
7	24.737	24.762	24.750	0.368	0.30	0.33
8	25.040	25.039	25.036	0.367	0.37	0.38
9	25.244	25.237	25.238	0.366	0.40	0.40
10	25.388	25.385	25.384	0.365	0.40	0.42
11	25.493	25.493	(25.492)	0.365	0.36	(0.37)
12	25.572			0.364		
13	25.633			0.363		
14	25.681			0.363		
15	25.720			0.363		
16	25.751			0.363		
17	25.777			0.363		
18	25.799			0.363		
19	25.817			0.363		
20	25.833			0.363		
21	25.846			0.363		
22	25.858			0.364		
23	25.868			0.364		
24	25.877			0.364		
25	25.884			0.364		
26	25.891			0.365		
27	25.897			0.365		
28	25.903			0.365		
29	25.908			0.365		
30	25.912			0.366		
31	25.916			0.366		
32	25.920			0.366		
33	25.923			0.367		
34	25.926			0.367		
35	25.929			0.367		
36	25.931			0.367		
37	25.933			0.368		
38	25.936			0.368		
39	25.938			0.368		
40	25.939			0.369		
…	…	…	…		…	…
∞	25.974	25.974	25.974			

Table 3. Resonance energies (E) and quantum defect (δ) of the $[3s^2 3p^3(^2D^{\circ}_{5/2})]nd$ Rydberg series originating from the $3s^2 3p^4\,^3P^{\circ}_0$ metastable state of the Cl^+ ions converging to the $3s^2 3p^3(^2D^{\circ}_{5/2})$ threshold of Cl^{2+}. The present results from the Modified atomic orbital theory (MAOT) are compared with the Dirac-Coulomb R-matrix (DCR) calculations of McLaughlin [5] and with the ALS experimental data of Hernández *et al*., [4]. The ALS experimental resonance energies are calibrated to ±0.013 eV. The energy limits is taken from the NIST tabulations of Ralchenko *et al*., [19]. $\sigma_1(^2D_{5/2}) = -0.789 \pm 0.048$; $\sigma_2(^2D_{5/2}) = 15.00$.

n	MAOT	DCR	ALS	MAOT	DCR	ALS
	E	E	E	δ	δ	δ
6	24.219	24.223	24.219	0.370	0.36	0.37
7	24.697	24.733		0.372	0.27	
8	25.001	24.999	(25.000)	0.371	0.38	(0.38)
9	25.205	25.198		0.370	0.40	
10	25.349	25.345		0.369	0.40	
11	25.455			0.368		
12	25.534			0.367		
13	25.595			0.367		
14	25.643			0.367		
15	25.682			0.366		
16	25.713			0.366		
17	25.739			0.366		
18	25.761			0.366		
19	25.779			0.367		
20	25.795			0.367		
21	25.808			0.367		
22	25.820			0.367		
23	25.830			0.367		
24	25.839			0.368		
25	25.846			0.368		
26	25.853			0.368		
27	25.859			0.368		
28	25.865			0.369		
29	25.870			0.369		
30	25.874			0.369		
31	25.878			0.370		
32	25.882			0.370		
33	25.885			0.370		
34	25.888			0.371		
35	25.891			0.371		
36	25.893			0.371		
37	25.895			0.371		
38	25.898			0.372		
39	25.900			0.372		
40	25.901			0.372		
…	…	…	…		…	…
∞	25.936	25.936	25.936			

Table 4. Resonance energies (E) and quantum defect (δ) of the $[3s^23p^3(^2P^\circ_{3/2})]nd$ Rydberg series originating from the $3s^23p^4\,^3P^\circ_2$ ground state of the Cl^+ ions converging to the $3s^23p^3(^2P^\circ_{3/2})$ threshold of Cl^{2+}. The present results from the Modified atomic orbital theory (MAOT) are compared with the Dirac-Coulomb R-matrix (DCR) calculations of McLaughlin [5] and with the ALS experimental data of Hernández *et al*., [4]. The ALS experimental resonance energies are calibrated to ±0.013 eV. The energy limits is taken from the NIST tabulations of Ralchenko *et al*., [19]. $\sigma_1(^2P_{3/2}) = -1.006 \pm 0.077$; $\sigma_2(^2P_{3/2}) = 15.00$.

n	MAOT	DCR	ALS	MAOT	DCR	ALS
	E	E	E	δ	δ	δ
6	25.749	25.755	(25.745)	0.459	0.46	(0.47)
7	26.246	26.253	26.246	0.469	0.45	0.47
8	26.562	26.576	26.564	0.471	0.45	0.46
9	26.774	26.780	26.778	0.471	0.44	0.45
10	26.923	26.927	26.928	0.470	0.44	0.43
11	27.031	27.035	27.031	0.469	0.43	0.47
12	27.113	27.115	(27.114)	0.468	0.44	(0.45)
13	27.176	27.178	27.175	0.467	0.42	0.48
14	27.225			0.467		
15	27.264			0.466		
16	27.296			0.466		
17	27.323			0.466		
18	27.345			0.466		
19	27.364			0.466		
20	27.379			0.466		
21	27.393			0.466		
22	27.405			0.466		
23	27.415			0.466		
24	27.424			0.467		
25	27.432			0.467		
26	27.439			0.467		
27	27.445			0.467		
28	27.450			0.468		
29	27.455			0.468		
30	27.460			0.468		
31	27.464			0.469		
32	27.467			0.469		
33	27.471			0.470		
34	27.474			0.470		
35	27.476			0.470		
36	27.479			0.471		
37	27.481			0.471		
38	27.483			0.471		
39	27.485			0.472		
40	27.487			0.472		
…	…	…	…		…	…
∞	27.522	27.522	27.522			

Table 5. Resonance energies (E, eV), quantum defect (δ) of the $[3s^2 3p^3(^2P^{\circ}_{3/2})]nd$ Rydberg series originating from the $3s^2 3p^4\ ^3P^{\circ}_1$ metastable state of the Cl^+ ions converging to the $3s^2 3p^3(^2P^{\circ}_{3/2})$ threshold of Cl^{2+}. The present results from the Modified atomic orbital theory (MAOT) are compared with the Dirac-Coulomb R-matrix (DCR) calculations of McLaughlin [5] and with the ALS experimental data of Hernández *et al.*, [4]. The ALS experimental resonance energies are calibrated to ±0.013 eV. The energy limits is taken from the NIST tabulations of Ralchenko *et al.*, [19]. $\sigma_1(^2P_{3/2}) = -1.018 \pm 0.076$; $\sigma_2(^2P_{3/2}) = 15.00$.

n	MAOT	DCR	ALS	MAOT	DCR	ALS
	E	E	E	δ	δ	δ
6	25.659	25.668	(25.660)	0.464	0.45	(0.45)
7	26.157	26.162	26.157	0.474	0.46	0.47
8	26.473	26.480	26.475	0.477	0.45	0.47
9	26.686	26.695	26.687	0.476	0.43	0.46
10	26.835	26.842	26.833	0.475	0.42	0.49
11	26.944			0.474		
12	27.025			0.473		
13	27.088			0.472		
14	27.138			0.472		
15	27.177			0.471		
16	27.209			0.471		
17	27.236			0.471		
18	27.258			0.471		
19	27.276			0.471		
20	27.292			0.471		
21	27.306			0.471		
22	27.318			0.471		
23	27.328			0.471		
24	27.337			0.472		
25	27.345			0.472		
26	27.351			0.472		
27	27.358			0.473		
28	27.363			0.473		
29	27.368			0.473		
30	27.373			0.474		
31	27.377			0.474		
32	27.380			0.475		
33	27.384			0.475		
34	27.387			0.475		
35	27.389			0.476		
36	27.392			0.476		
37	27.394			0.476		
38	27.396			0.477		
39	27.398			0.477		
40	27.400			0.477		
…	…	…	…		…	…
∞	27.435	27.435	27.435			

Table 6. Resonance energies (E) and quantum defect (δ) of the $[3s^23p^3(^2P^{\circ}_{3/2})]nd$ Rydberg series originating from the $3s^23p^4\,^3P^{\circ}_0$ metastable state of the Cl^+ ions converging to the $3s^23p^3(^2P^{\circ}_{3/2})$ threshold of Cl^{2+}. The present results from the Modified atomic orbital theory (MAOT) are compared with the Dirac-Coulomb R-matrix (DCR) calculations of McLaughlin [5] and with the ALS experimental data of Hernández *et al.*, [4]. The ALS experimental resonance energies are calibrated to ±0.013 eV. The energy limits is taken from the NIST tabulations of Ralchenko *et al.*, [19]. $\sigma_1(^2P_{3/2}) = -1.088 \pm 0.076$; $\sigma_2(^2P_{32}) = 15.00$.

n	MAOT	DCR	ALS	MAOT	DCR	ALS
	E	E	E	δ	δ	δ
6	25.603	25.635		0.493	0.44	
7	26.108	26.117	26.108	0.505	0.48	0.51
8	26.429	26.434	26.430	0.507	0.49	0.50
9	26.644	26.650	26.648	0.507	0.47	0.49
10	26.794	26.797		0.506	0.48	
11	26.904			0.504		
12	26.986			0.503		
13	27.050			0.502		
14	27.099			0.502		
15	27.139			0.501		
16	27.171			0.501		
17	27.198			0.501		
18	27.220			0.501		
19	27.239			0.501		
20	27.255			0.501		
21	27.268			0.501		
22	27.280			0.501		
23	27.290			0.502		
24	27.299			0.502		
25	27.307			0.502		
26	27.314			0.503		
27	27.320			0.503		
28	27.326			0.504		
29	27.331			0.504		
30	27.335			0.504		
31	27.339			0.505		
32	27.343			0.505		
33	27.346			0.506		
34	27.349			0.506		
35	27.352			0.507		
36	27.355			0.507		
37	27.357			0.507		
38	27.359			0.508		
39	27.361			0.508		
40	27.363			0.509		
…	…	…	…		…	…
∞	27.398	27.398	27.398			

Table 7. Resonance energies (E, eV), quantum defect (δ) of the $[3s^2 3p^3 (^2P^\circ_{1/2})]nd$ Rydberg series originating from the $3s^2 3p^4\,^1S^\circ_0$ metastable state of the Cl^+ ions converging to the $3s^2 3p^3 (^2P^\circ_{1/2})$ threshold of Cl^{2+}. The present results from the Modified atomic orbital theory (MAOT) are compared with the Dirac-Coulomb *R*-matrix (DCR) calculations of McLaughlin [5] and with the ALS experimental data of Hernández *et al.*, [4]. The ALS experimental resonance energies are calibrated to ±0.013 eV. The energy limits is taken from the NIST tabulations of Ralchenko *et al.*, [19]. $\sigma_1(^2P_{1/2}) = -0.262 \pm 0.015$; $\sigma_2(^2P_{1/2}) = 15.00$.

n	MAOT	DCR	ALS	MAOT	DCR	ALS
	E	E	E	δ	δ	δ
4	20.426	20.420	20.426	0.127	0.13	0.13
5	21.762	21.734	21.742	0.127	0.16	0.15
6	22.477	22.459	22.463	0.126	0.16	0.15
7	22.902	22.890	22.900	0.126	0.16	0.13
8	23.176	23.170	23.178	0.125	0.15	0.12
9	23.363	23.361		0.125	0.14	
10	23.496			0.125		
11	23.594			0.124		
12	23.668			0.124		
13	23.726			0.124		
14	23.771			0.124		
15	23.808			0.124		
16	23.838			0.124		
17	23.863			0.124		
18	23.884			0.124		
19	23.901			0.124		
20	23.916			0.124		
21	23.929			0.124		
22	23.940			0.124		
23	23.950			0.124		
24	23.959			0.124		
25	23.966			0.124		
26	23.973			0.125		
27	23.979			0.125		
28	23.984			0.125		
29	23.989			0.125		
30	23.993			0.125		
31	23.997			0.125		
32	24.000			0.125		
33	24.004			0.125		
34	24.007			0.125		
35	24.009			0.125		
36	24.012			0.125		
37	24.014			0.125		
…	…	…	…		…	…
∞	24.054	24.054	24.054			

Table 8. Resonance energies (E) and quantum defect (δ) of the $[3s^2 3p^3(^2D^{\circ}_{5/2})]nd$ series originating from the $3s^2 3p^4\,^1D_2$ metastable state of the Cl^+ ions converging to the $3s^2 3p^3(^2D^{\circ}_{5/2})$ threshold of Cl^{2+}. The present results from the Modified atomic orbital theory (MAOT) are compared with the Dirac-Coulomb R-matrix (DCR) calculations of McLaughlin [5] and with the ALS experimental data of Hernández *et al.*, [4]. The ALS experimental resonance energies are calibrated to ±0.013 eV. The energy limits is taken from the NIST tabulations of Ralchenko *et al.*, [19]. $\sigma_1(^2D_{5/2}) = -0.483 \pm 0.050$; $\sigma_2(^2D_{5/2}) = 15.00$.

n	MAOT	DCR	ALS	MAOT	DCR	ALS
	E	E	E	δ	δ	δ
6	22.979	22.969	22.979	0.232	0.25	0.27
7	23.427	23.392		0.233	0.32	
8	23.713	23.719	23.718	0.232	0.21	0.21
9	23.907	23.907	23.907	0.232	0.23	0.23
10	24.045	24.039	24.040	0.231	0.28	0.27
11	24.146	24.138	(24.152)	0.231	0.32	(0.27)
12	24.222			0.230		
13	24.281			0.230		
14	24.328			0.230		
15	24.366			0.230		
16	24.396			0.230		
17	24.421			0.229		
18	24.443			0.229		
19	24.461			0.229		
20	24.476			0.229		
21	24.489			0.229		
22	24.500			0.229		
23	24.510			0.229		
24	24.519			0.230		
25	24.526			0.230		
26	24.533			0.230		
27	24.539			0.230		
28	24.544			0.230		
29	24.549			0.230		
30	24.554			0.230		
31	24.558			0.230		
32	24.561			0.230		
33	24.564			0.230		
34	24.567			0.231		
35	24.570			0.231		
36	24.572			0.231		
37	24.575			0.231		
38	24.577			0.231		
39	24.579			0.231		
40	24.581			0.231		
…	…	…	…		…	…
∞	24.615	24.615	24.615			

Table 9. Resonance energies (E) and quantum defect (δ) of the $3s^2 3p^4(^1D_2)ns$ (j = 1/2 series originating from the $3s^2 3p^5\ ^2P^{\circ}_{1/2}$ metastable state of the Ar^+ ions converging to the $^1D_2$ threshold of Ar^{2+}. The present results from the Modified atomic orbital theory (MAOT) are compared with the Screening constant by unit nuclear charge (SCUNC) results of Sakho [11] are compared with the QB data of Covington *et al.*, [9]. The energy limits eV) is taken from the NIST tabulations of Ralchenko *et al.*, [17]. $\sigma_1(^1D_2) = -4.227 \pm 0.224$; $\sigma_2(^1D_2) = 16.00$.

n	MAOT	SCUNC	QB	MAOT	SCUNC	QB
	E	E	E	δ	δ	δ
8	27.830	27.830	27.830	1.672	1.673	1.673
9	28.169	28.173	28.173	1.695	1.682	1.682
10	28.400	28.401	28.401	1.696	1.689	1.688
11	28.561	28.561	28.561	1.689	1.694	1.692
12	28.678	28.676	28.677	1.679	1.697	1.695
13	28.765	28.763	28.763	1.670	1.699	1.698
14	28.831	28.829	28.829	1.662	1.700	1.699
15	28.883	28.881	28.881	1.656	1.701	1.701
16	28.925	28.923	28.923	1.652	1.701	1.702
17	28.958	28.956		1.649	1.700	
18	28.985	28.984		1.647	1.700	
19	29.008	29.007		1.647	1.698	
20	29.027	29.027		1.648	1.697	
21	29.044	29.043		1.649	1.695	
22	29.058	29.057		1.652	1.693	
23	29.070	29.069		1.655	1.691	
24	29.080	29.080		1.658	1.688	
25	29.089	29.089		1.662	1.686	
26	29.097	29.097		1.666	1.683	
27	29.104	29.104		1.670	1.680	
28	29.110	29.110		1.675	1.677	
29	29.116	29.116		1.679	1.674	
30	29.121	29.121		1.684	1.671	
31	29.126			1.689		
32	29.130			1.694		
33	29.133			1.699		
34	29.137			1.704		
35	29.140			1.708		
36	29.143			1.713		
37	29.145			1.718		
38	29.148			1.723		
39	29.150			1.727		
40	29.152			1.732		
…	…	…	…		…	…
∞	29.189	29.189	29.189			

Table 10. Resonance energies (E) and quantum defect (δ) of the $3s^23p^4$ ($^1D_2$)nd (j = 1/2 series originating from the $3s^23p^5\,^2P^{\circ}_{1/2}$ metastable state of the Ar^+ ions converging to the $3s^23p^4$($^1D_2$) threshold of Ar^{2+}. The present results from the Modified atomic orbital theory (MAOT) are compared with the Screening constant by unit nuclear charge (SCUNC) results of Sakho [11] are compared with the QB data of Covington *et al*., [9]. The energy limits eV) is taken from the NIST tabulations of Ralchenko *et al*., [17]. $\sigma_1(^1D_2) = -1.159 \pm 0.265$; $\sigma_2(^1D_2) = 16.00$.

n	MAOT	SCUNC	QB	MAOT	SCUNC	QB
	E	E	E	δ	δ	δ
8	28.211	28.211	28.211	0.540	0.540	0.540
9	28.428	28.426	28.426	0.543	0.555	0.554
10	28.581	28.578	28.576	0.543	0.563	0.574
11	28.691	28.689	28.691	0.542	0.568	0.546
12	28.775	28.772	28.773	0.541	0.571	0.562
13	28.838	28.837	28.837	0.540	0.573	0.568
14	28.889	28.887	28.887	0.539	0.573	0.572
15	28.929	28.928	28.928	0.538	0.573	0.574
16	28.961	28.960		0.538	0.572	
17	28.988	28.987		0.537	0.571	
18	29.011	29.010		0.537	0.570	
19	29.029	29.029		0.537	0.568	
20	29.045	29.045		0.537	0.567	
21	29.059	29.059		0.537	0.565	
22	29.071	29.071		0.537	0.563	
23	29.081	29.081		0.537	0.560	
24	29.090	29.090		0.537	0.558	
25	29.098	29.098		0.538	0.556	
26	29.105	29.105		0.538	0.553	
27	29.111	29.111		0.538	0.551	
28	29.117	29.117		0.538	0.548	
29	29.122	29.122		0.539	0.546	
30	29.126	29.126		0.539	0.543	
31	29.130			0.539		
32	29.134			0.540		
33	29.137			0.540		
34	29.140			0.540		
35	29.143			0.541		
36	29.146			0.541		
37	29.148			0.542		
38	29.150			0.542		
39	29.152			0.542		
40	29.154			0.543		
…	…	…	…		…	…
∞	29.189	29.189	29.189			

Table 11. Resonance energies (E) and quantum defect (δ) of the $3s^23p^4(^1D_2)nd$ (j = 3/2 series originating from the $3s^23p^5\,^2P^{\circ}_{1/2}$ metastable state of the Ar^+ ions converging to the $3s^23p^4(^1D_2)$ threshold of Ar^{2+}. The present results from the Modified atomic orbital theory (MAOT) are compared with the Screening constant by unit nuclear charge (SCUNC) results of Sakho [11] are compared with the QB data of Covington *et al.*, [9]. The energy limits eV) is taken from the NIST tabulations of Ralchenko *et al.*, [17]. $\sigma_1(^1D_2) = -1.159 \pm 0.265$; $\sigma_2(^1D_2) = 16.00$.

n	MAOT	SCUNC	QB	MAOT	SCUNC	QB
	E	E	E	δ	δ	δ
8	27.821	27.821	27.821	1.693	1.693	1.692
9	28.163	28.171	28.171	1.717	1.688	1.691
10	28.396	28.401	28.401	1.718	1.689	1.690
11	28.558	28.561	28.561	1.710	1.692	1.689
12	28.676	28.677	28.677	1.700	1.693	1.688
13	28.763	28.763	28.764	1.691	1.695	1.688
14	28.830	28.830	28.830	1.683	1.695	1.688
15	28.882	28.882	28.882	1.676	1.695	1.687
16	28.924	28.923	28.923	1.672	1.694	1.687
17	28.957	28.957		1.669	1.692	
18	28.985	28.984		1.667	1.691	
19	29.008	29.007		1.667	1.688	
20	29.027	29.027		1.668	1.686	
21	29.043	29.043		1.669	1.683	
22	29.057	29.057		1.672	1.679	
23	29.069	29.069		1.675	1.676	
24	29.080	29.080		1.678	1.672	
25	29.089	29.089		1.682	1.668	
26	29.097	29.097		1.686	1.663	
27	29.104	29.104		1.691	1.659	
28	29.110	29.111		1.695	1.655	
29	29.116	29.116		1.700	1.650	
30	29.121	29.121		1.705	1.645	
31	29.126			1.710		
32	29.130			1.715		
33	29.133			1.720		
34	29.137			1.725		
35	29.140			1.730		
36	29.143			1.735		
37	29.145			1.740		
38	29.148			1.745		
39	29.150			1.750		
40	29.152			1.754		
…	…	…	…		…	…
∞	29.189	29.189	29.189			

$3s^23p^4(^1D_2)ns$, nd (j = 1/2) and of the $3s^23p^4(^1D_2)nd$ (j = 3/2) series originating from the $3s^23p^5\ ^2P^{\circ}_{1/2}$ metastable state of the Ar II ions. Comparison indicate an excellent agreements between the present results from the Modified atomic orbital theory (MAOT) and both the Screening constant by unit nuclear charge (SCUNC) results [11] and the multichannel R-matrix QB technique which defines matrices Q and B in terms of asymptotic solutions [9]. These very good agreements are also observed comparing the resonance energies $3s^23p^4(^1D_2)ns$, nd (j = 1/2) series originating from the $3s^23p^5\ ^2P^{\circ}_{3/2}$ ground state of the Ar II ions. For both **Tables 9-12**, the QB data are limited to n = 16 and the SCUNC values to n = 30. High lying MAOT data are tabulated up to n = 40 with a constant quantum defect along each series. **Table 13** and **Table 14** quote respectively resonance energies of the $3s^23p^4(^1D_2)nd$ (j = 1/2)and of the $3s^23p^4(^1D_2)ns$ (j = 3/2) series originating from the $3s^23p^5\ ^2P^{\circ}_{3/2}$ ground state of the Ar II ions. Here again, the agreements between the present MAOT results and both SCUNC of Sakho [11] and QB results of Covington *et al*., [9] are very good. **Table 15** presents resonance energies of the $3s^23p^4\ (^1D_2)nd$ (j = 3/2) series originating from the $3s^23p^5\ ^2P^{\circ}_{3/2}$ ground state of the Ar II ions. In this Table, an uncertain QB data [9] is quoted at (28.774 eV) for the $3s^23p^4(^1D_2)10d$ level. For this level, the MOAT prediction is at 28.735 eV to be compared to the SCUNC forecast at 28.734 eV. Subsequently, the QB data at (28.774 eV) associated with a quantum defect equal to (0.422) is less precise. For this level, both the MAOT and SCUNC [11] predictions associated with the quantum defects 0.721 and 0.724 are preferable. Therefore, it should be underlined that the SCUNC calculations are more precise than the MOAT calculations. This is due mainly to the fact that, the SCUNC formalism is a development of $1/Z$ taking implicitly into account more relativistic effects than the MAOT formalism witch is a simple development on $1/n$. In addition, in the SCUNC formalism, great accuracy are obtained when performing the analytical formula for each atomic system [11]. In the present work, the same Formula (6) is used for both Cl II, Ar II and Kr II in contrast with the work of Sakho [11] where the resonance energy expression for the Ar II ions is different to that of the Kr II ions. **Table 16** and **Table 17** list natural widths of the $[3s^23p^4(^1D_2)]ns$, nd (j = 1/2) (**Table 16**) and of the $[3s^23p^4(^1D_2)]ns$, nd (j = 3/2) (**Table 17**) series originating from the $3s^23p^5\ ^2P^{\circ}_{1/2}$ metastable state of Ar^+ ions. It can be seen that the present MAOT data agree well with both the SCUNC results [11] and QB data [9]. It should be mentioned again that the SCUNC calculations are more precise than the MOAT calculations for the reason explained above. **Table 18** lists resonance energies and quantum defect of the $[4s^24p^4\ (^1D_2)]nd$ series originating from the $4s^24p^5\ ^2P^{\circ}_{3/2}$ ground state of the Kr II ions. Comparisons indicate very good agreements between the present results from the MAOT formalism and both the SCUNC calculations [11] up to n = 30 and ALS measurements of [10] up to n = 13. In this iable, two uncertain ALS data are quoted for the $[4s^24p^4(^1D_2)]12d$ and $[4s^24p^4(^1D_2)]13d$ levels respectively at (25.880 eV) and (25.926 eV). The

Table 12. Resonance energies (E) and quantum defect (δ) of the $3s^23p^4(^1D_2)ns$ ($j = 1/2$ series originating from the $3s^23p^5\,^2P^{\circ}_{3/2}$ ground state of the Ar^+ ions converging to the $3s^23p^4(^1D_2)$ threshold of Ar^{2+}. The present results from the Modified atomic orbital theory (MAOT) are compared with the Screening constant by unit nuclear charge (SCUNC) results of Sakho [11] are compared with the QB data of Covington *et al*., [9]. The energy limits eV) is taken from the NIST tabulations of Ralchenko *et al*., [17]. $\sigma_1(^1D_2) = -4.234 \pm 0.224$; $\sigma_2(^1D_2) = 16.00$.

n	MAOT	SCUNC	QB	MAOT	SCUNC	QB
	E	E	E	δ	δ	δ
8	28.007	28.007	28.007	1.674	1.674	1.673
9	28.346	28.351	28.351	1.698	1.681	1.682
10	28.577	28.579	28.579	1.699	1.688	1.688
11	28.739	28.739	28.739	1.691	1.694	1.692
12	28.856	28.854	28.854	1.681	1.698	1.696
13	28.943	28.941	28.941	1.672	1.701	1.698
14	29.009	29.007	29.007	1.664	1.702	1.700
15	29.061	29.059	29.059	1.658	1.702	1.701
16	29.103	29.101	29.100	1.654	1.702	1.702
17	29.136	29.135		1.651	1.700	
18	29.163	29.162		1.649	1.698	
19	29.186	29.185		1.649	1.696	
20	29.205	29.205		1.650	1.693	
21	29.222	29.221		1.652	1.690	
22	29.236	29.235		1.654	1.686	
23	29.248	29.247		1.657	1.682	
24	29.258	29.258		1.660	1.678	
25	29.267	29.267		1.664	1.673	
26	29.275	29.275		1.668	1.668	
27	29.282	29.282		1.672	1.663	
28	29.288	29.289		1.677	1.658	
29	29.294	29.294		1.682	1.653	
30	29.299	29.299		1.686	1.647	
31	29.304			1.691		
32	29.308			1.696		
33	29.311			1.701		
34	29.315			1.706		
35	29.318			1.711		
36	29.321			1.716		
37	29.323			1.720		
38	29.326			1.725		
39	29.328			1.730		
40	29.330			1.734		
…	…	…	…		…	…
∞	29.367	29.367	29.367			

Table 13. Resonance energies (E) and quantum defect (δ) of the $3s^23p^4(^1D_2)nd$ (j = 1/2 series originating from the $3s^23p^5\,^2P^{\circ}_{3/2}$ ground state of the Ar^+ ions converging to the $3s^23p^4(^1D_2)$ threshold of Ar^{2+}. The present results from the Modified atomic orbital theory (MAOT) are compared with the Screening constant by unit nuclear charge (SCUNC) results of Sakho [11] are compared with the QB data of Covington *et al.*, [9]. The energy limits eV) is taken from the NIST tabulations of Ralchenko *et al.*, [17]. $\sigma_1(^1D_2) = -1.159 \pm 0.265$; $\sigma_2(^1D_2) = 16.00$.

n	MAOT	SCUNC	QB	MAOT	SCUNC	QB
	E	E	E	δ	δ	δ
8	28.389	28.389	28.389	0.540	0.540	0.540
9	28.606	28.603	28.603	0.543	0.560	0.554
10	28.759	28.755	28.754	0.543	0.567	0.574
11	28.869	28.867	28.869	0.542	0.572	0.546
12	28.953	28.950	28.951	0.541	0.575	0.562
13	29.016	29.014	29.014	0.540	0.578	0.568
14	29.067	29.065	29.065	0.539	0.581	0.572
15	29.107	29.105	29.105	0.538	0.583	0.574
16	29.139	29.138		0.538	0.585	
17	29.166	29.165		0.537	0.587	
18	29.189	29.187		0.537	0.588	
19	29.207	29.206		0.537	0.589	
20	29.223	29.223		0.537	0.590	
21	29.237	29.236		0.537	0.589	
22	29.249	29.248		0.537	0.589	
23	29.259	29.259		0.537	0.587	
24	29.268	29.268		0.537	0.585	
25	29.276	29.276		0.538	0.581	
26	29.283	29.283		0.538	0.577	
27	29.289	29.289		0.538	0.572	
28	29.295	29.295		0.538	0.566	
29	29.300	29.300		0.539	0.559	
30	29.304	29.304		0.539	0.551	
31	29.308			0.539		
32	29.312			0.540		
33	29.315			0.540		
34	29.318			0.540		
35	29.321			0.541		
36	29.324			0.541		
37	29.326			0.542		
38	29.328			0.542		
39	29.330			0.542		
40	29.332			0.543		
…	…	…	…		…	…
∞	29.367	29.367	29.367			

Table 14. Resonance energies (E) and quantum defect (δ) of the $3s^23p^4(^1D_2)ns$ ($j = 3/2$ series originating from the $3s^23p^5\,^2P^\circ_{3/2}$ ground state of the Ar^+ ions converging to the $3s^23p^4(^1D_2)$ threshold of Ar^{2+}. The present results from the Modified atomic orbital theory (MAOT) are compared with the Screening constant by unit nuclear charge (SCUNC) results of Sakho [11] are compared with the QB data of Covington *et al.*, [9]. The energy limits eV) is taken from the NIST tabulations of Ralchenko *et al.*, [17]. $\sigma_1(^1D_2) = -4.294 \pm 0.224$; $\sigma_2(^1D_2) = 16.00$.

n	MAOT	SCUNC	QB	MAOT	SCUNC	QB
	E	E	E	δ	δ	δ
8	27.999	27.999	27.999	1.693	1.693	1.692
9	28.341	28.348	28.348	1.717	1.692	1.691
10	28.574	28.578	28.579	1.718	1.692	1.690
11	28.736	28.739	28.739	1.710	1.693	1.689
12	28.854	28.855	28.855	1.700	1.694	1.688
13	28.941	28.941	28.941	1.691	1.694	1.688
14	29.008	29.008	29.098	1.683	1.695	1.688
15	29.060	29.060	29.060	1.676	1.695	1.687
16	29.102	29.101	29.101	1.672	1.695	1.687
17	29.135	29.135		1.669	1.695	
18	29.163	29.162		1.667	1.695	
19	29.186	29.185		1.667	1.694	
20	29.205	29.205		1.668	1.694	
21	29.221	29.221		1.669	1.693	
22	29.235	29.235		1.672	1.692	
23	29.247	29.247		1.675	1.691	
24	29.258	29.258		1.678	1.690	
25	29.267	29.267		1.682	1.689	
26	29.275	29.275		1.686	1.688	
27	29.282	29.282		1.691	1.687	
28	29.288	29.288		1.695	1.686	
29	29.294	29.294		1.700	1.684	
30	29.299	29.299		1.705	1.683	
31	29.304			1.710		
32	29.308			1.715		
33	29.311			1.720		
34	29.315			1.725		
35	29.318			1.730		
36	29.321			1.735		
37	29.323			1.740		
38	29.326			1.745		
39	29.328			1.750		
40	29.330			1.754		
…	…	…	…		…	…
∞	29.367	29.367	29.367			

Table 15. Resonance energies (E, eV) and quantum defect (δ) of the $3s^23p^4(^1D_2)nd$ (j = 3/2 series originating from the $3s^23p^5\,^2P^{\circ}_{3/2}$ ground state of the Ar^+ ions converging to the $3s^23p^4(^1D_2)$ threshold of Ar^{2+}. The present results from the Modified atomic orbital theory (MAOT) are compared with the Screening constant by unit nuclear charge (SCUNC) results of Sakho [11] are compared with the QB data of Covington *et al.*, [9]. The energy limits eV) is taken from the NIST tabulations of Ralchenko *et al.*, [17]. $\sigma_1(^1D_2) = -1.575 \pm 0.265$; $\sigma_2(^1D_2) = 16.00$.

n	MAOT	SCUNC	QB	MAOT	SCUNC	QB
	E	E	E	δ	δ	δ
8	28.341	28.341	28.341	0.717	0.717	0.716
9	28.573	28.573	28.573	0.721	0.721	0.720
10	28.735	28.734	(28.774)	0.721	0.724	(0.422)*
11	28.852	28.851	28.850	0.720	0.727	0.738
12	28.939	28.939	28.937	0.718	0.729	0.745
13	29.006	29.006	29.004	0.717	0.729	0.744
14	29.059	29.058	29.047	0.715	0.729	0.744
15	29.100	29.100	29.099	0.714	0.728	0.744
16	29.134	29.134		0.713	0.727	
17	29.162	29.162		0.713	0.725	
18	29.185	29.185		0.713	0.722	
19	29.204	29.204		0.712	0.720	
20	29.221	29.221		0.712	0.718	
21	29.235	29.235		0.713	0.716	
22	29.247	29.247		0.713	0.714	
23	29.257	29.257		0.713	0.713	
24	29.267	29.267		0.714	0.712	
25	29.275	29.275		0.714	0.712	
26	29.282	29.282		0.715	0.713	
27	29.288	29.288		0.715	0.715	
28	29.294	29.294		0.716	0.719	
29	29.299	29.299		0.717	0.723	
30	29.304	29.303		0.717	0.729	
31	29.308			0.718		
32	29.311			0.719		
33	29.315			0.719		
34	29.318			0.720		
35	29.321			0.721		
36	29.323			0.722		
37	29.326			0.722		
38	29.328			0.723		
39	29.330			0.724		
40	29.332			0.724		
…	…	…	…		…	…
∞	29.367	29.367	29.367			

*This line is not well identified.

Table 16. Natural widths (Γ, meV) of the $[3s^23p^4(^1D_2)]ns$, nd (j = 1/2) series originating from the $3s^23p^5\,^2P^{\circ}_{1/2}$ metastable state of Ar^+ ions. The present results from the Modified atomic orbital theory (MAOT) are compared with the Screening constant by unit nuclear charge (SCUNC) results of Sakho [11] are compared with the QB data of Covington *et al.*, [9]. For: $[4s^24p^4(^1D_2)]$ ns: $\sigma_1(^1D_2) = -5.494 \pm 0.010$; $\sigma_2(^1D_2) = 17.989 \pm 0.010$. For: $[4s^24p^4(^1D_2)]nd$: $\sigma_1(^1D_2) = -0.168 \pm 0.010$; $\sigma_2(^1D_2) = 17.998 \pm 0.010$.

n	$[4s^24p^4(^1D_2)]ns$ series			$[4s^24p^4(^1D_2)]nd$ series		
	MAOT	SCUNC	QB	MAOT	SCUNC	QB
	Γ	Γ	Γ	Γ	Γ	Γ
8	103.5	103.4	103.4	0.112	0.110	0.110
9	64.9	64.8	64.8	0.072	0.070	0.070
10	43.4	43.0	43.0	0.048	0.047	0.050
11	30.4	30.0	30.0	0.034	0.033	0.040
12	22.1	21.7	21.8	0.024	0.024	0.030
13	16.5	16.2	16.3	0.018	0.018	0.020
14	12.7	12.4	12.5	0.014	0.014	0.020
15	9.9	9.8	9.8	0.011	0.011	0.020
16	7.8	7.8	7.8	0.008	0.009	
17	6.3	6.4		0.007	0.008	
18	5.1	5.3		0.005	0.006	
19	4.2	4.5		0.004	0.005	
20	3.5	3.8		0.004	0.005	
21	2.9	3.3		0.003	0.004	
22	2.5	2.9		0.003	0.003	
23	2.1	2.5		0.002	0.003	
24	1.8	2.2		0.002	0.003	
25	1.5	2.0		0.002	0.002	

Table 17. Natural widths (Γ, meV) of the $[3s^23p^4(^1D_2)]ns$, nd (j = 3/2) series originating from the $3s^23p^5\,^2P^{\circ}_{1/2}$ metastable state of Ar^+ ions. The present results from the Modified atomic orbital theory (MAOT) are compared with the Screening constant by unit nuclear charge (SCUNC) results of Sakho [11] are compared with the QB data of Covington *et al.*, [9]. For: $[4s^24p^4(^1D_2)]$ ns: $\sigma_1(^1D_2) = -0.670 \pm 0.010$; $\sigma_2(^1D_2) = 18.038 \pm 0.010$. For: $[4s^24p^4(^1D_2)]$ nd: $\sigma_1(^1D_2) = -1.399 \pm 0.010$; $\sigma_2(^1D_2) = 17.827 \pm 0.010$.

n	$[4s^24p^4(^1D_2)]ns$ series			$[4s^24p^4(^1D_2)]nd$ series		
	MAOT	SCUNC	QB	MAOT	SCUNC	QB
	Γ	Γ	Γ	Γ	Γ	Γ
8	0.44	0.44	0.44	25.7		25.7
9	0.22	0.22	0.22	18.1		18.1
10	0.13	0.11	0.13	12.9		33.8
11	0.08	0.06	0.08	9.3		8.5

Continued

12	0.05	0.03	0.08	6.9		3.8
13	0.03	0.02	0.04	5.2		5.3
14	0.02	0.01	0.02	4.0		4.4
15	0.01	0.01	0.02	3.1		3.6
16				2.5		
17				2.1		
18				1.7		
19				1.4		
20				1.2		
21				1.0		
22				0.9		
23				0.8		
24				0.7		
25				0.6		

Table 18. Resonance energies (E) and quantum defect (δ) of the $[4s^24p^4(^1D_2)]nd$ series originating from the $4s^24p^5\,^2P^\circ_{3/2}$ ground state of the Kr^+ ions converging to the $[4s^24p^4(^1D_2)]$ threshold of Kr^{2+}. The present results from the Modified atomic orbital theory (MAOT) are compared with the Screening constant by unit nuclear charge (SCUNC) results of Sakho [11] are compared with the ALS experimental data of Hinojoha *et al.*, [10]. The ALS resonance energies are calibrated to ±30 meV and quantum defects are estimated to within an error of 20%. The energy limits is taken from the NIST tabulations of Ralchenko *et al.*, [18]. Here $\sigma_1(^1D_2) = -0.719 \pm 0.116$; $\sigma_2(^1D_2) = 34.00$.

n	MAOT	SCUNC	ALS	MAOT	SCUNC	ALS
	E	E	E	δ	δ	δ
5	24.342	24.342	24.342	−0.387	−0.387	−0.385
6	24.882	24.878	24.878	−0.386	−0.375	−0.370
7	25.220	25.215	25.217	−0.387	−0.369	−0.370
8	25.444	25.439	25.441	−0.389	−0.366	−0.370
9	25.600	25.596	25.598	−0.390	−0.365	−0.360
10	25.713	25.710	25.712	−0.390	−0.365	−0.358
11	25.798	25.796	25.796	−0.391	−0.365	−0.345
12	25.863	25.861	(25.880)	−0.391	−0.366	(−0.671)
13	25.913	25.912	(25.926)	−0.391	−0.367	(−0.663)
14	25.954	25.953		−0.391	−0.368	
15	25.987	25.987		−0.390	−0.369	
16	26.014	26.014		−0.390	−0.370	
17	26.037	26.037		−0.390	−0.371	
18	26.056	26.056		−0.389	−0.372	
19	26.072	26.072		−0.389	−0.373	
20	26.086	26.086		−0.389	−0.373	
21	26.098	26.098		−0.388	−0.374	
22	26.108	26.108		−0.388	−0.374	
23	26.118	26.117		−0.387	−0.374	
24	26.125	26.125		−0.387	−0.374	

Continued

25	26.133	26.132		−0.387	−0.374	
26	26.139	26.139		−0.386	−0.374	
27	26.144	26.144		−0.386	−0.374	
28	26.149	26.149		−0.385	−0.373	
29	26.154	26.154		−0.385	−0.373	
30	26.158	26.158		−0.385	−0.372	
31	26.162			−0.384		
32	26.165			−0.384		
33	26.168			−0.383		
34	26.171			−0.383		
35	26.174			−0.383		
36	26.176			−0.382		
37	26.178			−0.382		
38	26.180			−0.382		
39	26.182			−0.381		
40	26.184			−0.381		
…	…	…	…		…	…
∞	29.367	29.367	29.367			

associated ALS quantum defects are equal to (−0.671) and (−0.663) respectively. For the same levels, the MAOT and SCUNC calculations [11] are respectively at 25.863 eV and 25.861 eV for the $[4s^24p^4(^1D_2)]12d$ state and at 25.913 eV and 25.912 eV for the $[4s^24p^4(^1D_2)]13d$ state. Constant quantum defects are tabulated for the MAOT and SCUNC predictions [11] respectively at −0.31 and −0.37. So the MAOT and SCUNC estimations can be considered as the accurate data for the $[4s^24p^4(^1D_2)]12d$ and $[4s^24p^4(^1D_2)]13d$ resonances. **Table 19** quotes resonance energies and quantum defect of the $4s^24p^4(^3P_2,^3P_1)]ns$ and $4s^24p^4(^3P_1)]ns$ series originating from the $4s^24p^5\,^2P^{\circ}_{1/2}$ metastable state of the Kr II ions. For the $4s^24p^4(^3P_2)]ns$ series, comparisons indicate good agreements between theory and experiments. It should be underlined the very good agreements for n = 13 - 20. This may enlighten the accuracy of the uncertain ALS measurement [10] listed into parenthesis. For the $4s^24p^4(^3P_1)]ns$ series only one ALS data at 23.996 eV is quoted. New MAOT values from n = 14 to 40 are tabulated with a constant quantum defect about 0.42. In **Table 20**, resonance energies and quantum defect of the $4s^24p^4(^3D_2)]ns$, $n$dseries originating from the $4s^24p^5\,^2P^{\circ}_{1/2}$ metastable state of the Kr II ions are listed. Here again, the MAOT data agree very well with the ALS data of Hinojoha *et al.*, [10]. It should be underlined the excellent agreements between theory and experiments for the $4s^24p^4(^3D_2)]8s$ and $4s^24p^4(^3D_2)]9s$ levels. For these states, both the MAOT and ALS work provide the same values respectively equal to 24.650 eV and 24.842 eV. The excellent agreement for the quantum defects can also be mentioned, 0.20 for both theory and experiments. **Table 21** presents resonance energies and quantum defect for the

Table 19. Resonance energies (E) and quantum defect (δ) of the $4s^24p^4(^3P_2,^3P_1)]ns$ series originating from the $4s^24p^5\,^2P^\circ_{1/2}$ metastable state of the Kr^+ ions converging to the $[4s^24p^4(^1D_2)]$ threshold of Kr^{2+}. The present results from the Modified atomic orbital theory (MAOT) are compared with the Screening constant by unit nuclear charge (SCUNC) results of Sakho [11] are compared with the ALS experimental data of Hinojoha *et al.*, [10]. The ALS resonance energies are calibrated to ±30 meV and quantum defects are estimated to within an error of 20%.The energy limits is taken from the NIST tabulations of Ralchenko *et al.*, [18]. $\sigma_1(^3P_2) = -1.438 \pm 0.104$; $\sigma_2(^3P_2) = 34.00$; $\sigma_1(^3P_1) = -0.863 \pm 0.138$; $\sigma_2(^3P_1) = 34.00$.

n	$4s^24p^4(^3P_2)]ns$				$4s^24p^4(^3P_1)]ns$			
	MAOT	ALS	MAOT	ALS	MAOT	ALS	MAOT	ALS
	E	E	δ	δ	E	E	δ	δ
11	23.910	(23.906)	−0.771	(−0.716)				
12	23.969	23.969	−0.765	−0.779				
13	24.016	24.016	−0.762	−0.791				
14	24.053	(24.059)	−0.761	(−0.940)	23.957		0.418	
15	24.084	24.083	−0.761	−0.730	23.996	23.996	0.419	0.403
16	24.109	24.109	−0.762	−0.774	24.028		0.420	
17	24.131	(24.129)	−0.762	(−0.686)	24.054		0.420	
18	24.148	(24.147)	−0.763	(−0.707)	24.076		0.420	
19	24.164	(24.162)	−0.764	(−0.659)	24.094		0.420	
20	24.177	(24.176)	−0.764	(−0.731)	24.110		0.420	
21	24.188		−0.765		24.124		0.420	
22	24.198		−0.765		24.135		0.420	
23	24.207		−0.765		24.145		0.419	
24	24.214		−0.766		24.154		0.419	
25	24.221		−0.766		24.162		0.419	
26	24.227		−0.766		24.169		0.419	
27	24.232		−0.766		24.175		0.419	
28	24.237		−0.766		24.180		0.419	
29	24.242		−0.766		24.185		0.418	
30	24.246		−0.766		24.190		0.418	
31	24.249		−0.766		24.194		0.418	
32	24.252		−0.765		24.197		0.418	
33	24.255		−0.765		24.201		0.418	
34	24.258		−0.765		24.204		0.418	
35	24.260		−0.765		24.206		0.418	
36	24.263		−0.765		24.209		0.418	
37	24.265		−0.764		24.211		0.418	
38	24.267		−0.764		24.213		0.418	
39	24.269		−0.764		24.215		0.418	
40	24.270		−0.763		24.217		0.418	
…								
∞	24.303	24.303			24.252	24.252		

Table 20. Resonance energies (E) and quantum defect (δ) of the $4s^24p^4(^3D_2)]ns$, nd series originating from the $4s^24p^5\,^2P^{\circ}_{1/2}$ metastable state of the Kr^+ ions converging to the $[4s^24p^4(^1D_2)]$ threshold of Kr^{2+}. The present results from the Modified atomic orbital theory (MAOT) are compared with the Screening constant by unit nuclear charge (SCUNC) results of Sakho [11] are compared with the ALS experimental data of Hinojoha *et al.*, [10]. The ALS resonance energies are calibrated to ±30 meV and quantum defects are estimated to within an error of 20%. The energy limits is taken from the NIST tabulations of Ralchenko *et al.*, [18]. $\sigma_1(^1D_2) = -0.414 \pm 0.116$; $\sigma_2(^1D_2) = 34.00$ for $4s^24p^4(^3D_2)]ns$. $\sigma_1(^1D_2) = -0.698 \pm 0.116$; $\sigma_2(^1D_2) = 34.00$ for $4s^24p^4(^3D_2)]nd$.

n	$4s^24p^4(^3D_2)]ns$				$4s^24p^4(^3D_2)]nd$			
	MAOT	ALS	MAOT	ALS	MAOT	ALS	MAOT	ALS
	E	E	δ	δ	E	E	δ	δ
6	23.927	23.927	0.200	0.200	24.214	24.214	−0.371	−0.375
7	24.368	(24.366)	0.200	(0.205)	24.553	24.551	−0.369	−0.371
8	24.650	24.650	0.200	0.204)	24.778	24.775	−0.370	−0.371
9	24.842	24.842	0.200	0.201	24.935	24.933	−0.371	−0.375
10	24.978	-	0.199	-	25.049	25.047	−0.372	−0.379
11	25.079	25.082	0.199	0.152	25.134	25.132	−0.372	−0.363
12	25.154	25.158	0.199	0.139	25.199	25.196	−0.373	−0.349
13	25.213		0.198		25.251	25.248	−0.373	−0.364
14	25.259		0.198		25.292		−0.373	
15	25.297		0.198		25.325		−0.373	
16	25.327		0.198		25.352		−0.373	
17	25.352		0.198		25.375		−0.373	
18	25.373		0.198		25.394		−0.373	
19	25.391		0.198		25.410		−0.373	
20	25.406		0.198		25.424		−0.373	
21	25.419		0.198		25.436		−0.373	
22	25.431		0.198		25.446		−0.372	
23	25.440		0.198		25.455		−0.372	
24	25.449		0.198		25.463		−0.372	
25	25.457		0.198		25.470		−0.372	
26	25.463		0.198		25.477		−0.371	
27	25.469		0.198		25.482		−0.371	
28	25.475		0.198		25.487		−0.371	
29	25.479		0.198		25.492		−0.371	
30	25.484		0.198		25.496		−0.370	
31	25.488		0.198		25.500		−0.370	
32	25.491		0.198		25.503		−0.370	
33	25.494		0.198		25.506		−0.370	
34	25.497		0.198		25.509		−0.369	
35	25.500		0.198		25.511		−0.369	
36	25.503		0.198		25.514		−0.369	
37	25.505		0.199		25.516		−0.369	
38	25.507		0.199		25.518		−0.368	
39	25.509		0.199		25.520		−0.368	
40	25.511		0.199		25.522		−0.368	
…								
∞	25.545	25.545			25.555	25.555		

Table 21. Resonance energies (E) and quantum defect (δ) of the $4s^24p^4(^3D_2, ^1S_0)]ns$, nd series of the Kr^+ ions. The present results from the Modified atomic orbital theory (MAOT) are compared with the Screening constant by unit nuclear charge (SCUNC) results of Sakho [11] are compared with the ALS experimental data of Hinojoha *et al.*, [10]. The ALS resonance energies are calibrated to ±30 meV and quantum defects are estimated to within an error of 20%. $\sigma_1(^1D_2) = -0.785 \pm 0.116$; $\sigma_2(^1D_2) = 34.00$; $\sigma_1(^1S_0) = -0.811 \pm 0.116$; $\sigma_2(^1S_0) = 34.00$.

n	$4s^24p^5\,^2P^\circ_{1/2} \rightarrow 4s^24p^4(^1S_0)]ns$				$4s^24p^5\,^2P^\circ_{3/2} \rightarrow 4s^24p^4(^1S_0)]nd$			
	MAOT	ALS	MAOT	ALS	MAOT	ALS	MAOT	ALS
	E	E	δ	δ	E	E	δ	δ
4	23.738	23.738	0.357	0.358				
5	25.315	25.312	0.358	0.360	25.965	(25.947)	0.369	(0.385)
6	26.132	26.124	0.355	0.368	26.780	26.780	0.380	0.379
7	26.608	26.602	0.353	0.371	27.261	(27.261)	0.381	(0.379)
8	26.910	26.904	0.352	0.376	27.566	27.566	0.381	0.376
9	27.112	27.108	0.351	0.377	27.771	27.771	0.379	0.378
10	27.255	(27.261)	0.351	(0.303)	27.915	27.914	0.378	0.381
11	27.360	27.356	0.351	0.400	28.021	28.020	0.378	0.383
12	27.439	27.435	0.351	0.412	28.100	28.099	0.377	0.381
13	27.500	(27.495)	0.351	(0.435)	28.161	(28.160)	0.377	(0.394)
14	27.548	(27.544)	0.352	(0436)	28.210	(28.208)	0.376	(0.394)
15	27.586		0.352		28.249	(28.247)	0.376	(0.418)
16	27.618		0.353		28.280		0.376	
17	27.644		0.354		28.306		0.376	
18	27.665		0.354		28.328		0.376	
19	27.683		0.355		28.346		0.376	
20	27.699		0.356		28.362		0.376	
21	27.712		0.356		28.375		0.377	
22	27.724		0.357		28.387		0.377	
23	27.734		0.358		28.397		0.377	
24	27.743		0.358		28.405		0.377	
25	27.750		0.359		28.413		0.378	
26	27.757		0.359		28.420		0.378	
27	27.763		0.360		28.426		0.378	
28	27.769		0.361		28.432		0.379	
29	27.774		0.361		28.437		0.379	
30	27.778		0.362		28.441		0.379	
31	27.782		0.362		28.445		0.379	
32	27.786		0.363		28.449		0.380	
33	27.789		0.363		28.452		0.380	
34	27.792		0.364		28.455		0.380	
35	27.795		0.364		28.458		0.381	
36	27.797		0.365		28.460		0.381	
37	27.799		0.365		28.462		0.381	
38	27.802		0.366		28.465		0.382	
39	27.804		0.366		28.467		0.382	
40	27.805		0.366		28.468		0.382	
…								
∞	27.840	27.840			28.503	28.503		

$4s^2 4p^4 (^3D_2, {}^1S_0)]ns$, nd series of the Kr II ions. Here again, the good agreements between the present MAOT and ALS data [10] may enlighten the accuracy of the uncertain ALS measurement listed into parenthesis. Overall, for both the Cl II, Ar II and Kr II ions, it is demonstrated in this paper the possibilities to reproduce excellently high ALS measurements from single MAOT analytical expression. This is the main strength of the present work.

4. Conclusion

Accurate high lying resonance energy up to $n = 40$ is reported applying the Modified atomic orbital theory. For both the Cl II, Ar II and Kr II ions investigated, a single formula has been established to reproduce with a very good accuracy high experimental measurements such as those performed at the Advanced Light Source at Lawrence Berkeley National Laboratory. A huge number of results are tabulated as useful reference data for interpreting atomic spectra from astrophysical objects containing chlorine, argon and krypton elements.

Conflicts of Interest

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

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