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Modified Atomic Orbital Calculations of Energy and Width of the 2pns $^1P^\circ$ and 2pnd$^1P^\circ$ Rydbergs Series of Be-like N^{3+}, O^{4+}, F^{5+} and Ne^{6+} Ions

Research Article

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Abstract. We report accurate energy resonances and natural widths belonging to the $1s^22s^2\ ^1S_0 \rightarrow (2pnl)\ ^1P^\circ$ and $1s^22s\ 2p\ ^3P_0 \rightarrow 1s^22p\ [^2P^\circ]\ np\ ^3P$ transitions in the Photoionization spectra of the Be-like N^{3+}, O^{4+}, F^{5+} and Ne^{6+} ions. Calculations are performed in the framework of the *Modified Orbital Atomic Theory* (MAOT). Excellent agreements are obtained with available experimental and theoretical literature data. The present calculations provide benchmark data for the diagnostic and for the modeling of astrophysical and laboratory plasmas.

Keywords. Energy resonances; Widths; Modified atomic orbital theory; Rydberg series; Photoionization

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1. Introduction

The study of Photoionization of atoms and ions is of great importance for understanding fundamental processes occurring in astrophysical systems and laboratory plasma. Consequently, it is very challenging to provide photoionization parameters in connection with the Opacity Project. Quantitative measurements of photoionization of ions are carried out using synchrotron radiations providing high accurate measurements to benchmark state-of-the-art theoretical quantum mechanical methods. Ions of great interest are those of carbon (C^{2+}, C^{3+}, C^{4+}), of nitrogen (N^{2+}, N^{3+}, N^{4+}) and of oxygen (O^{2+}, O^{3+}, O^{4+}) known to contribute to the opacity in the atmospheres of the central stars of planetary nebulas [1, 2]. For Be-like systems, previous measurements incorporate Be atom [3], and Be-like ions such as B^+ [4], C^{2+} [5], N^{3+} and O^{4+} [6]. On the view point of theory, the R-matrix approach has been applied to report resonance energies and widths of the 2pns $^1P^{\circ}$ and 2pnd$^1P^{\circ}$ Rydberg series of O^{4+} [7], F^{5+} [8] and Ne^{6+}ions [9]. In addition, the *Screening Constant by Unit Nuclear Charge* (SCUNC) [10] to present accurate resonance energies and widths of the 2pns $^1P^{\circ}$ and 2pnd$^1P^{\circ}$ Rydberg series of Be-like ions ($Z = 8-18$). In general, most of the *ab initio* and experimental methods employed in the investigations of the Rydberg series of atomic systems are based on the determination of the Photoionization cross section. Specific codes consuming time are also required to succeed on obtaining accurate resonance energies and widths. The goal of the present work is report accurate energy resonances and natural widths of the 2pns $^1P^{\circ}$ and 2pnd$^1P^{\circ}$ Rydbergs series of Be-like N^{3+}, O^{4+}, F^{5+} and Ne^{6+} without calculation and Photoionization cross section neither using a specific code. In this purpose, we apply the *Modified Atomic Orbital Theory* (MAOT) [11–14]. The organization of the present work is as follows. Section 2 presents a brief outline of the theoretical method. In Section 3 we display the results obtained and comparison is done with available literature data. Summary and conclusion are given in Section 4.

2. Theory

2.1 Brief Description of the MAOT Formalism

In the framework of the *Modified Atomic Orbital Theory* (MAOT), the total energy of a ($\nu\ell$)-given orbital is expressed in the form [11–14]

$$E(\upsilon\ell) = -\frac{[Z-\sigma(\ell)]^2}{\upsilon^2}. \tag{2.1}$$

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

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

For the $(N\ell, n\ell')^{2S+1}L^{\pi}$ doubly excited states, the total energy of an atomic system of many M electrons is expressed as follows:

$$E = -\sum_{i=1}^{M} \frac{\left[Z-\sigma_i(^{2S+1}L^{\pi})\right]^2}{\nu_i^2}. \tag{2.2}$$

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 [12] (in Rydberg units)

$$E_n = E_\infty - \frac{1}{n^2}\left\{Z - \sigma_1(^{2S+1}L_J) - \sigma_2(^{2S+1}L_J)\times\frac{1}{n} - \sigma_2^{\alpha}(^2P^0_{3/2}, {}^1D_2)\times(n-m)\times(n-q)\sum_k \frac{1}{f_k(n,m,q,s)}\right\}^2. \tag{2.3}$$

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 ($s = \frac{1}{2}$), E_∞ is the energy value of the series limit generally determined from 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 eq. (2.3) 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

$$E_n = E_\infty - \frac{RZ^2}{(n-\delta)^2}.$$

2.2 Energy Resonances of the 2p*n*s ^{1}P° and 2p*n*d ^{1}P° Series

Using eq. (2.3) we find

- For the $2s^2\ ^1S_0 \rightarrow 2pns\ ^1P^\circ$ transitions

$$E_n = E_\infty - \frac{1}{n^2}\left\{Z - \sigma_1 - \sigma_2 \times \frac{1}{n} + \sigma_2 \times (n-m) \times (n-q) \times \left[\frac{1}{(n+q-m+s)^4} + \frac{1}{(n+q-m+s+1)^5} + \frac{1}{(n+q+s-1)^3} + \frac{1}{(n+m+s-1)^4} + \frac{1}{(n+q+s-1)^4} + \frac{1}{(n+q-m+s)^5}\right]\right\}^2. \quad (2.4)$$

- For the $2s^2\ ^1S_0 \rightarrow 2pnd\ ^1P^\circ$ transitions

$$E_n = E_\infty - \frac{1}{n^2}\left\{Z - \sigma_1 - \sigma_2 \times \frac{1}{n} - \sigma_2 \times (n-m) \times (n-q) \times \left[\frac{1}{(n+q+s-1)^3} + \frac{1}{(n+m+s-1)^3} + \frac{1}{(n+m+s)^3} + \frac{1}{(n+m+s-1)^4} + \frac{1}{(n+q+s-1)^3} + \frac{1}{(n+q-s-1)^4}\right]\right\}^2. \quad (2.5)$$

The σ_i-screening constants in eqs. (2.4) and (2.5) are evaluated using the Electron Beam Ion Trap energy resonances measured by Simon *et al*. [15] for the following transitions in N^{3+}

- $2s^2\ ^1S_0 \rightarrow 2p5s\ ^1P^\circ$ (m = 5): E (2p5s ^{1}P°) = 77.85 ± 0.02 eV
- $2s^2\ ^1S_0 \rightarrow 2p6s\ ^1P^\circ$ (q = 6): E (2p6s ^{1}P°) = 80.89 ± 0.03 eV
- $2s^2\ ^1S_0 \rightarrow 2p5d\ ^1P^\circ$ (m = 5): E (2p5d ^{1}P°) = 78.89 ± 0.02 eV
- $2s^2\ ^1S_0 \rightarrow 2p6d\ ^1P^\circ$ (q = 6): E (2p6d ^{1}P°) = 81.49 ± 0.02 eV.

The energy limits is at 87.473 eV for the 2pnl series. Using these experimental data, eqs. (2.4) and (2.5) give respectively

- σ_1(s) = 2.984 ± 0.035 and σ_2(s) = – 0.944 ± 0.154.
- σ_1(d) = 2.984 ± 0.017 and σ_2(d) = 0.225 ± 0.061.

2.3 Natural Widths of the 2p*n*s ^{1}P° and 2p*n*d ^{1}P° Series

The resonance widths of the 2p*n*s ^{1}P° and 2p*n*d ^{1}P° doubly excited states of the Be-like ions investigated are given by (in Rydberg units)

- For the $2s^2\ {}^1S_0 \rightarrow 2pns\ {}^1P^\circ$ transitions

$$\Gamma_n = \frac{1}{n^2}\left\{Z - \sigma'_1 \times \left(\frac{Z}{Z_0}\right) - \sigma'_2 \times \frac{1}{n} + \sigma'_2 \times \left(\frac{Z}{Z_0}\right) \times (n-m) \times (n-q) \times \left[\frac{1}{(n+q-m+s+1)^3} + \frac{1}{(n+q-m+s+1)^5} + \frac{1}{(n+q+s)^4} + \frac{1}{(n+m+s)^5} + \frac{1}{(n+q+s)^3} + \frac{1}{(n+q-m+s)^4}\right]\right\}^2. \quad (2.6)$$

- For the $2s^2\ {}^1S_0 \rightarrow 2pnd\ {}^1P^\circ$ transitions

$$\Gamma_n = \frac{1}{n^2}\left\{Z - \sigma'_1 \times \left(\frac{Z}{Z_0}\right) + \sigma'_2 \times \left(\frac{Z}{Z_0}\right) \times \frac{1}{n} + \sigma'_2 \times \left(\frac{Z}{Z_0}\right)^2 \times (n-m) \times (n-q) \times \left[\frac{1}{(n+q-m+s)^3} + \frac{1}{(n+q-m+s)^3} + \frac{1}{(n+q-m+s+1)^4} + \frac{1}{(n+q-m+s+1)^4} + \frac{1}{(n+q-m+s)^4} + \frac{1}{(n+q-m+s)^5}\right]\right\}^2. \quad (2.7)$$

In eq. (2.6) and (2.7), Z_0 denotes the nuclear charge of the Be-like ion used to determine empirically the the σ'_i-screening constants. Using the Advanced Light Source results of Schippers *et al*. [4] for the following transitions in B^+ (so $Z_0 = 5$):

- $2s^2\ {}^1S_0 \rightarrow 2p4s\ {}^1P^\circ$ (m = 4): Γ (2p4s ^{1}P°) = 0.220 ± 0.001 eV
- $2s^2\ {}^1S_0 \rightarrow 2p5s\ {}^1P^\circ$ (q = 5): Γ (2p5s ^{1}P°) = 0.106 ± 0.007 eV
- $2s^2\ {}^1S_0 \rightarrow 2p4d\ {}^1P^\circ$ (m = 4): Γ (2p4d ^{1}P°) = 0.034 ± 0.002 eV
- $2s^2\ {}^1S_0 \rightarrow 2p5d\ {}^1P^\circ$ (q = 5): Γ (2p5d ^{1}P°) = 0.016 ± 0.002 eV.

Using these experimental data, Eqs. (2.6) gives respectively with $Z_0 = 5$ for B^+:

- $\sigma'_1(s) = 4.828 \pm 0.068$ and $\sigma'_2(s) = -1.346 \pm 0.268$.
- $\sigma'_1(d) = 4.871 \pm 0.00x$ and $\sigma'_2(d) = -0.032 \pm 0.00x$.

3. Results and Discussion

The results obtained in this work for energy positions (E) and quantum defects (δ) of the 2p*n*s ^{1}P° and 2p*n*d ^{1}P° Rydberg series of the Be-like N^{3+}, O^{4+}, F^{5+} and Ne^{6+} ion investigated are listed in Tables 1–3. Table 4 shows a comparison the present Modified atomic orbital theory (MAOT) for the calculations of energy positions of the 2p*n*s ^{1}P° and 2p*n*d ^{1}P° Rydberg series of the Be-like N^{3+} ion compared with theoretical results from R-matrix calculations from Opacity Project (TOP) database as quoted in Simon *et al*. [15], *Multi-configuration Dirac-Fock* (MCDF) calculations of Simon *et al*. [15], *Cowan Atomic Structure Code* (CATS) results as quoted in Simon *et al*. [15], *Screening Constant by Unit Nuclear Charge* (SCUNC) calculations of Sakho *et al*. [17] and with experimental data from *Electron Beam Ion Trap* (EBIT) measurements of Simon *et al*. [15] and with *Merged-Beam* (MB) measurement of Bizau *et al*. [6].

Table 1. Energy positions (E) and quantum defects (δ) of the 2pns ^{1}P° and 2pnd^{1}P° Rydberg series of the Be-like N^{3+} and O^{4+} ions. The energy positions and the widths are expressed in eV. The energy value of the series limit is taken from NIST [16]

	2pns ^{1}P°				2pnd^{1}P°			
	N^{3+}		O^{4+}		N^{3+}		O^{4+}	
n	E	δ	E	δ	E	δ	E	δ
5	77.851	0.244	-	-	78.8912	-0.037	-	-
6	80.891	0.249	115.782	0.201	81.4909	-0.032	116.530	-0.026
7	82.693	0.252	118.535	0.203	83.0684	-0.030	119.003	-0.024
8	83.846	0.253	120.301	0.203	84.0963	-0.029	120.613	-0.023
9	84.628	0.253	121.501	0.203	84.8028	-0.029	121.719	-0.023
10	85.182	0.252	122.354	0.202	85.3089	-0.030	122.512	-0.024
11	85.589	0.251	122.980	0.202	85.6838	-0.030	123.098	-0.024
12	85.896	0.250	123.454	0.201	85.9691	-0.031	123.545	-0.025
13	86.134	0.248	123.821	0.199	86.1913	-0.032	123.892	-0.026
14	86.322	0.247	124.111	0.198	86.3676	-0.033	124.168	-0.027
15	86.473	0.246	124.345	0.198	86.5099	-0.034	124.391	-0.027
16	86.596	0.245	124.535	0.197	86.6263	-0.035	124.573	-0.028
17	86.698	0.244	124.692	0.196	86.7229	-0.035	124.724	-0.028
18	86.783	0.244	124.824	0.196	86.8038	-0.036	124.851	-0.029
19	86.854	0.243	124.935	0.195	86.8723	-0.036	124.958	-0.029
20	86.915	0.243	125.030	0.195	86.9307	-0.036	125.049	-0.029
21	86.968	0.243	125.111	0.195	86.9811	-0.036	125.128	-0.029
22	87.013	0.243	125.182	0.195	87.0247	-0.036	125.196	-0.029
23	87.053	0.243	125.243	0.195	87.0628	-0.036	125.256	-0.029
24	87.087	0.244	125.297	0.195	87.0962	-0.036	125.308	-0.028
25	87.118	0.244	125.344	0.196	87.1257	-0.035	125.354	-0.028
26	87.1448	0.245	125.386	0.196	87.1518	-0.034	125.3949	-0.027
27	87.1689	0.246	125.4235	0.197	87.1751	-0.033	125.4313	-0.027
28	87.1904	0.247	125.4570	0.198	87.1960	-0.033	125.4640	-0.026
29	87.2097	0.248	125.4870	0.198	87.2147	-0.031	125.4933	-0.025
30	87.2271	0.249	125.5140	0.199	87.2316	-0.030	125.5197	-0.024
...	...		...		...			
∞	87.473		125.897		87.473		125.897	

Table 2. Energy positions (E) and quantum defects (δ) of the 2pns ^{1}P° and 2pnd^{1}P° Rydberg series of the Be-like F^{5+} and Ne^{6+} ions. The energy positions and the widths are expressed in eV. The energy value of the series limit is taken from NIST [16]

	2pns ^{1}P°				2pnd^{1}P°			
	F^{5+}		Ne^{6+}		F^{5+}		Ne^{6+}	
n	E	δ	E	δ	E	δ	E	δ
7	160.6724	0.170	209.1208	0.146	161.2331	-0.020	209.7740	-0.017
8	163.1823	0.170	212.5042	0.146	163.5559	-0.019	212.9395	-0.017
9	164.8900	0.170	214.8085	0.146	165.1510	-0.019	215.1127	-0.017
10	166.1038	0.169	216.4479	0.145	166.2932	-0.020	216.6687	-0.017
11	166.9971	0.168	217.6554	0.145	167.1389	-0.020	217.8206	-0.017
12	167.6736	0.168	218.5702	0.144	167.7824	-0.021	218.6970	-0.018
13	168.1980	0.167	219.2798	0.143	168.2833	-0.021	219.3793	-0.018
14	168.6127	0.166	219.8413	0.142	168.6809	-0.022	219.9208	-0.019
15	168.9464	0.165	220.2932	0.142	169.0017	-0.023	220.3577	-0.019
16	169.2188	0.164	220.6623	0.141	169.2642	-0.023	220.7152	-0.020
17	169.4440	0.164	220.9675	0.141	169.4819	-0.024	221.0116	-0.020
18	169.6325	0.163	221.2229	0.140	169.6643	-0.024	221.2600	-0.021
19	169.7916	0.163	221.4388	0.140	169.8186	-0.024	221.4703	-0.021
20	169.9273	0.163	221.6228	0.140	169.9505	-0.024	221.6498	-0.021
21	170.0439	0.163	221.7810	0.140	170.0639	-0.024	221.8042	-0.021
22	170.1449	0.163	221.9179	0.140	170.1622	-0.024	221.9382	-0.021
23	170.2328	0.163	222.0373	0.140	170.2480	-0.024	222.0550	-0.021
24	170.3100	0.163	222.1420	0.140	170.3233	-0.024	222.1575	-0.020
25	170.3780	0.163	222.2343	0.140	170.3898	-0.023	222.2480	-0.020
26	170.4382	0.164	222.3160	0.140	170.4487	-0.023	222.3283	-0.020
27	170.4919	0.164	222.3889	0.141	170.5012	-0.022	222.3998	-0.019
28	170.5398	0.165	222.4540	0.141	170.5482	-0.022	222.4638	-0.019
29	170.5829	0.166	222.5125	0.142	170.5904	-0.021	222.5213	-0.018
30	170.6217	0.166	222.5652	0.143	170.6285	-0.020	222.5731	-0.017
...	...	...	...		...		...	
∞	171.172		223.313		171.172		223.313	

Table 3. Energy positions (E) and quantum defects (δ) of the 2pns ^{1}P° and 2pnd^{1}P° Rydberg series of the Be-like Na^{7+} and Mg^{8+} ions. The energy positions and the widths are expressed in eV. The energy value of the series limit is taken from NIST [16]

	2pns ^{1}P°				2pnd^{1}P°			
	Na^{7+}		Mg^{8+}		Na^{7+}		Mg^{8+}	
n	E	δ	E	δ	E	δ	E	δ
8	268.2445	0.128	330.4762	0.114	268.7414	-0.015	331.0348	-0.013
9	271.2348	0.128	334.2417	0.114	271.5821	-0.015	334.6321	-0.013
10	273.3635	0.128	336.9237	0.114	273.6156	-0.015	337.2071	-0.013
11	274.9323	0.127	338.9010	0.113	275.1210	-0.015	339.1131	-0.013
12	276.1215	0.126	340.4004	0.112	276.2663	-0.016	340.5633	-0.014
13	277.0443	0.125	341.5643	0.112	277.1579	-0.016	341.6921	-0.014
14	277.7747	0.125	342.4858	0.111	277.8654	-0.017	342.5879	-0.015
15	278.3627	0.124	343.2278	0.110	278.4363	-0.017	343.3106	-0.015
16	278.8430	0.124	343.8341	0.110	278.9036	-0.017	343.9022	-0.015
17	279.2405	0.123	344.3358	0.110	279.2908	-0.018	344.3925	-0.016
18	279.5730	0.123	344.7557	0.109	279.6154	-0.018	344.8034	-0.016
19	279.8541	0.122	345.1107	0.109	279.8901	-0.018	345.1512	-0.016
20	280.0938	0.122	345.4134	0.109	280.1246	-0.018	345.4481	-0.016
21	280.2999	0.122	345.6737	0.109	280.3265	-0.018	345.7036	-0.016
22	280.4783	0.122	345.8991	0.109	280.5015	-0.018	345.9251	-0.016
23	280.6339	0.122	346.0957	0.109	280.6541	-0.018	346.1184	-0.016
24	280.7703	0.122	346.2680	0.109	280.7881	-0.018	346.2880	-0.016
25	280.8906	0.123	346.4200	0.109	280.9063	-0.018	346.4377	-0.016
26	280.9972	0.123	346.5547	0.109	281.0112	-0.017	346.5704	-0.015
27	281.0921	0.123	346.6747	0.110	281.1046	-0.017	346.6887	-0.015
28	281.1770	0.124	346.7820	0.110	281.1882	-0.016	346.7946	-0.014
29	281.2533	0.124	346.8783	0.111	281.2633	-0.016	346.8896	-0.014
30	281.3220	0.125	346.9652	0.111	281.3311	-0.015	346.9754	-0.013
...	...	...	...		...		...	
∞	282.2976		348,1988		282.2976		348.1988	

Table 4. Present MAOT energy positions (E, in eV) of the 2pns ^{1}P° and 2pnd^{1}P° Rydberg series of the Be-like N^{3+} ion compared with literature data

Levels	MAOT	SCUNC	NIST	TOP	MCDF	CATS	EBIT, exp.	MB, exp.
2p5s ^{1}P°	77.85	77.93	77.93	77.93	77.73	76.1	77.85 (2)	77.72 (5)
2p6s ^{1}P°	80.89	80.95		80.81	80.71	79.3	80.89 (3)	
2p7s ^{1}P°	82.69	82.73		82.63	82.54	81.1	82.70 (5)	
2p8s ^{1}P°	83.85	83.87						
2p9s ^{1}P°	84.63	84.65						
2p10s ^{1}P°	85.18	85.19						
2p11s ^{1}P°	85.59	85.60						
2p12s ^{1}P°	85.90	85.90						
2p13s ^{1}P°	86.13	86.14						
2p14s ^{1}P°	86.32	86.33						
2p15s ^{1}P°	86.47	86.48						

SCUNC, Screening constant by unit nuclear charge results of sakho *et al*. [17]
TOP, R-matrix calculations from Opacity Project (TOP) database as quoted in Simon *et al*. [15]
MCDF, Multi-configuration Dirac-Fock (MCDF) calculations of Simon *et al*. [15]
CATS, Cowan Atomic Structure Code (CATS) as quoted in Simon *et al*. [15]
EBIT, exp. Electron Beam Ion Trap experiments of Simon *et al*. [15]
MB, exp. Merged-Beam experiments of Bizau *et al*. [6].

Table 5. Energy positions (E, eV), widths (Γ, eV) effective quantum number (n^*) of the of the 2pns ^{1}P° Rydberg series of the Be-like O^{4+} ion

	MAOT		SCUNC		R-matrix	
n	E	n^*	E	n^*	E	n^*
6	115.782	5.799	115.676	5.770	115.680	5.825
7	118.535	6.797	118.474	6.770	118.365	6.812
8	120.301	7.797	120.266	7.772	120.110	7.804
9	121.501	8.797	121.479	8.774	121.302	8.800
10	122.354	9.798	122.338	9.776	122.150	9.797
11	122.980	10.798	122.969			
12	123.454	11.799	123.446			
13	123.821	12.801	123.814			
14	124.111	13.802	124.106			
15	124.345	14.802	124.340			
16	124.535	15.803	124.531			
17	124.692	16.804	124.689			
18	124.824	17.804	124.821			
19	124.935	18.805	124.933			
20	125.030	19.805	125.028			
21	125.111	20.805	125.109			
22	125.182	21.805	125.180			
23	125.243	22.805	125.242			
24	125.297	23.805	125.296			
25	125.344	24.804	125.343			

MAOT, Modified atomic orbital theory, present calculations
SCUNC, Screening constant by unit nuclear charge results of sakho *et al*. [15]
R-matrix, calculations of Kim and Manson [8]

Table 6. Energy positions (E, eV), widths (Γ, eV) effective quantum number (n^*) of the of the 2pnd^{1}P° Rydberg series of the Be-like O^{4+} ion

	MAOT		SCUNC		R-matrix	
n	E	n^*	E	n^*	E	n^*
6	116.530	6.026	116.544	6.030	116.351	6.034
7	119.003	7.024	119.015	7.030	118.816	7.032
8	120.613	8.023	120.622	8.030	120.421	8.031
9	121.719	9.023	121.726	9.030	121.523	9.031
10	122.512	10.024	122.516	10.030	122.301	10.030
11	123.098	11.024	123.102			
12	123.545	12.025	123.547			
13	123.892	13.026	123.894			
14	124.168	14.027	124.170			
15	124.391	15.027	124.392			
16	124.573	16.028	124.574			
17	124.724	17.028	124.725			
18	124.851	18.029	124.851			
19	124.958	19.029	124.958			
20	125.049	20.029	125.050			
21	125.128	21.029	125.129			
22	125.196	22.029	125.197			
23	125.256	23.029	125.256			
24	125.308	24.028	125.309			
25	125.354	25.028	125.355			

MAOT, Modified atomic orbital theory, present calculations
SCUNC, Screening constant by unit nuclear charge results of sakho *et al*. [15]
R-matrix, calculations of Kim *et al.* [18]

Table 7. Energy positions (E, eV), widths (Γ, eV) effective quantum number (n^*) of the of the 2pns ^{1}P° Rydberg series of the Be-like F^{5+} ion

	MAOT		SCUNC		R-matrix	
n	E	n^*	E	n^*	E	n^*
7	160.672	6.830	160.567	6.796	160.606	6.818
8	163.182	7.830	163.119	7.779	163.128	7.818
9	164.890	8.830	164.849	8.801	164.843	8.818
10	166.104	9.831	166.056	9.803	166.061	9.817
11	166.997	10.832	166.976			
12	167.674	11.832	167.659			
13	168.198	12.833	168.186			
14	168.613	13.834	168.603			
15	168.946	14.835	168.938			
16	169.219	15.836	169.212			
17	169.444	16.836	169.438			
18	169.632	17.837	169.627			
19	169.792	18.837	169.787			
20	169.927	19.837	169.924			
21	170.044	20.837	170.041			
22	170.145	21.837	170.142			
23	170.233	22.837	170.230			
24	170.310	23.837	170.308			
25	170.378	24.837	170.376			

MAOT, Modified atomic orbital theory, present calculations
SCUNC, Screening constant by unit nuclear charge results of sakho *et al*. [15]
R-matrix, calculations of Kim and Kim [19]

Table 8. Energy positions (E, eV), widths (Γ, eV) effective quantum number (n^*) of the of the 2pnd^{1}P° Rydberg series of the Be-like F^{5+} ion

	MAOT		SCUNC		R-matrix	
n	E	n^*	E	n^*	E	n^*
6	157.664	6.022	157.681	6.025	157.665	6.028
7	161.233	7.020	161.247	7.025	161.222	7.027
8	163.556	8.019	163.566	8.025	163.538	8.026
9	165.151	9.019	165.158	9.024	165.129	9.025
10	166.293	10.020	166.298	10.024	166.269	10.025
11	167.139	11.020	167.142			
12	167.782	12.021	167.785			
13	168.283	13.021	168.285			
14	168.681	14.022	168.682			
15	169.002	15.023	169.003			
16	169.264	16.023	169.265			
17	169.482	17.024	169.483			
18	169.664	18.024	169.665			
19	169.819	19.024	169.819			
20	169.950	20.024	169.9512			
21	170.064	21.024	170.065			
22	170.162	22.024	170.163			
23	170.248	23.024	170.249			
24	170.323	24.024	170.324			
25	170.390	25.023	170.391			

MAOT, Modified atomic orbital theory, present calculations
SCUNC, Screening constant by unit nuclear charge results of sakho *et al*. [15]
R-matrix, calculations of Kim and Kim [19]

Table 9. Energy positions (E, eV), widths (Γ, eV) effective quantum number (n^*) of the of the 2pns ^{1}P° Rydberg series of the Be-like Ne^{6+} ion

	MAOT		SCUNC		R-matrix	
n	E	n^*	E	n^*	E	n^*
7	209.121	6.830	208.968	6.817	209.005	6.852
8	212.504	7.830	212.411	7.820	212.375	7.846
9	214.809	8.830	214.748	8.822	214.680	8.844
10	216.448	9.831	216.405	6.817		
11	217.655	10.832	217.624			
12	218.570	11.832	218.546			
13	219.280	12.833	219.261			
14	219.841	13.834	219.826			
15	220.293	14.835	220.281			
16	220.662	15.836	220.652			
17	220.968	16.836	220.959			
18	221.223	17.837	221.215			
19	221.439	18.837	221.432			
20	221.623	19.837	221.617			
21	221.781	20.837	221.776			
22	221.918	21.837	221.914			
23	222.037	22.837	222.034			
24	222.142	23.837	222.139			
25	222.234	24.837	222.231			

MAOT, Modified atomic orbital theory, present calculations
SCUNC, Screening constant by unit nuclear charge results of Sakho *et al*. [15]
R-matrix, calculations of Kim and Kwon [20]

Table 10. Energy positions (E, eV), widths (Γ, eV) effective quantum number (n^*) of the of the 2pnd^{1}P° Rydberg series of the Be-like Ne^{6+} ion

	MAOT		SCUNC		R-matrix	
n	E	n^*	E	n^*	E	n^*
7	209.774	7.017	209.789	7.021	209.682	7.022
8	212.939	8.017	212.951	8.021	212.843	8.021
9	215.113	9.017	215.120	9.021	215.012	9.021
10	216.669	10.017	216.674			
11	217.821	11.017	217.824			
12	218.697	12.018	218.699			
13	219.379	13.018	219.381			
14	219.921	14.019	219.922			
15	220.358	15.019	220.359			
16	220.715	16.020	220.716			
17	221.012	17.020	221.012			
18	221.260	18.021	221.261			
19	221.470	19.021	221.471			
20	221.650	20.021	221.650			
21	221.804	21.021	221.805			
22	221.938	22.021	221.939			
23	222.055	23.021	222.056			
24	222.158	24.020	222.158			
25	222.248	25.020	222.249			

MAOT, Modified atomic orbital theory, present calculations
SCUNC, Screening constant by unit nuclear charge results of Sakho *et al*. [15]
R-matrix, calculations of Kim and Kwon [20]

Comparison indicates good agreement between the calculations and between the MOAT results and the experimental data. It should be underlined the good agreements between the SCUNC and the MAOT values for the high levels $n = 8 - 15$. Tables 5 and 6 list energy resonances and effective quantum number (n^*) of the 2pns ^{1}P° (Table 5) and 2pnd ^{1}P° (Table 6) Rydberg series of the Be-like O^{4+} ion. Here, the present MOAT results are compared with the available SCUNC values of Sakho *et al*. [15] and with the R-matrix calculations of Kim and Manson [8] and of Kim *et al*. [18]. Up to the high level $n = 25$, it is seen that the present MOAT calculations agree well with the SCUNC predictions [15]. The maximum energy deviation is less than 0.07 eV for $6 \le n \le 10$ and less than 0.02 eV for $11 \le n \le 25$. Besides, comparisons with the R-matrix calculations [8, 15], show good agreement as the energy deviations have never overrun 0.3 eV for $6 \le n \le 10$. Tables 7 and 8 show the present MAOT energy resonances and effective quantum number of the 2pns ^{1}P° (Table 7) and 2pnd ^{1}P° (Table 8) Rydberg series of the Be-like F^{5+} ion compared the SCUNC values of Sakho *et al*. [15] and with the R-matrix calculations of Kim *et al*. [18]. Here again, comparisons indicate good agreements between the calculations. It should be underlined that the MOAT calculations match more with the SCUNC predictions [15] up to $n = 25$. As far as the R-matrix calculations are concerned, it can be seen that the energy deviations with are less than 0.07 eV for $6 \le n \le 10$ for the 2pns ^{1}P° states as quoted in Table 7 and less 0.03 eV for $6 \le n \le 10$ for the 2pnd ^{1}P° states as listed in Table 8. This indicated the good agreements between the present MAOT data and the R-matrix calculations of Kim *et al*. [18]. Tables 9 and 10 show the present MAOT energy resonances and effective quantum number of the 2pns ^{1}P° (Table 9) and 2pnd ^{1}P° (Table 10) Rydberg series of the Be-like Ne^{6+} ion compared the SCUNC values of Sakho *et al*. [15] and with the R-matrix calculations of Kim and Kwon [20]. Comparisons show good agreements between the MAOT calculations and both the SCUNC predictions [15] up to $n = 25$ and the R-matrix calculations [20]. But, it should be mentioned the slight discrepancies between the MAOT data and the R-matrix calculations of Kim and Kwon [20] as the energy deviation range between 0.116 eV and 0.129 eV for the 2pns ^{1}P° (Table 9) and between 0.092 eV and 0.541 eV for the 2pnd ^{1}P° (Table 10) for $7 \le n \le 10$. Overral, the slight discrepancies between the present MAOT data and the R-matrix calculations [8, 18, 20] are due to the simplicity of the formalism where relativistic and electron correlation effects are not incorporated explicitly in the analytical formula (2.4) and (2.6). But, it should be underlined the soft procedure of the present formalism leading to accurate results up to high n in contrast with the R-matrix method based on the DARC codes and as a result, the use of this method require more consuming time than the very soft MAOT formalism.

4. Conclusions

Accurate energy resonances for the (2pnl) ^{1}P° states of the Be-like N^{3+} ions along with energy resonances of the $1s^2 2p$ [^{2}P°] np ^{3}P series of the Be-like N^{3+} and O^{4+} ions are reported along with energy positions of the $1s^2 2s2p^6(^2S_{1/2})$ np ^{1}P° Rydberg series of Ar^{8+} converging to the $1s^2 2s2p^6(^2S_{1/2})$ series limit in Ar^{9+}. Calculations are performed using the Screening Constant by Unit Nuclear Charge (SCUNC) method for high lying states. Very good agreements with available experimental and theoretical literature data are found. The present calculations provide benchmark data for the diagnostic and for the modeling of astrophysical and laboratory plasmas.

Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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