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Theoretical calculation of photoionization cross sections of B-like ions: N^{2+}, O^{3+} and F^{4+}*

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There can be found some notable discrepancies with regard to the resonance structures when R-matrix calculations from the Opacity Project and other sources are compared with recent absolute experimental measurements of Bizau *et al* [*Astron. Astrophts.* **439** 387 (2005)] for B-like ions N^{2+}, O^{3+} and F^{4+}. We performed close-coupling calculations based on the R-matrix formalism for the photoionizations of ions mentioned above both for the ground states and first excited states in the near threshold regions. The present results are compared with experimental ones given by Bizau *et al* and earlier theoretical ones. Excellent agreement is obtained between our theoretical results and the experimental photoionization cross sections. The present calculations show a significant improvement over the previous theoretical results.

Keywords: photoionization, N^{2+}, O^{3+}, F^{4+}, resonance
PACC: 3280F, 3280D

1. Introduction

Absolute photoionization (PI) cross sections of atoms and ions are required to model many physical systems, such as astrophysical or laboratory plasma and the upper atmosphere. Multiply charged ions of low-Z elements such as carbon, nitrogen, and oxygen have received much attention in a number of theoretical and experimental studies due to their importance in astrophysics. For B-like ions, as a part of the Opacity Project (OP),[1] Fernley *et al* [2] calculated the PI cross sections of the N^{2+}, O^{3+} and F^{4+} using the R-matrix method. Nahar and Pradhan[3] and Nahar[4,5] calculated the PI cross sections of the ions of C, N, and O under the Iron Project (IP).[6] Experimentally, Champeaux *et al*[7] measured absolute photoionization cross sections of O^{3+} in the ground state and several metastable states. In order to compare their experimental results with theoretical ones, Champeaux *et al* also performed multiconfiguration Dirac-Fock and relativistic R-matrix calculations.

The accuracy of the data for atomic and ionic photoionization cross sections is very important for practical application. Recently, in order to test the R-matrix calculations of the Opacity Projects, Bizau *et al* [8] measured absolute photoionization cross sections for the light multiply charged ions of astrophysical relevance: N^{2+}, N^{3+}, O^{3+}, O^{4+}, F^{3+}, F^{4+} and Ne^{4+}. In the experiment they used the merged-beam technique in combination with the synchrotron radiation from an undulator at the storage ring ASTRID with ions produced by an ECR ion source. Although there have been many theoretical studies for these ions, very significant discrepancy between the experimental data and previous R-matrix calculations is observed concerning the spectral structure of some ions studied. To improve the accuracy of theoretical calculation, we calculate photoionization cross sections of some B-like ions mentioned above in this paper.

2. Theoretical methods

The photoionization cross sections are calculated using the R-matrix method[9] and the corresponding programs.[10] In the R-matrix calculation, the wavefunction of the $N+1$ electron system is given by

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$$\Psi_k(X_1,\ldots,X_{N+1}) = \hat{A}\sum_{ij} c_{ijk}\,\Phi_i(X_1,\ldots,X_N,$$

$$\hat{r}_{N+1}\sigma_{N+1})u_{ij} + \sum_j d_{jk}\phi_j(X_1,\ldots,X_{N+1}) \qquad (1)$$

where $\hat{A}$ is the antisymmetrization operator to take into account the exchange effect between the target electrons and the free electron. X_i denotes the spatial (r_i) and the spin (s_i) coordinates of the i-th electron. The functions $u_{ij}(r)$ in the first sum construct the basis sets for the continuum wave functions of the free electron, and Φ_i are the coupling between the target states and the angular and the spin parts of the free electron. The correlation functions in the second sum are constructed by the square integrable orbitals to account for the correlation effects, which is not adequately considered because of the cutoff in the first sum. The square integrable orbitals are expressed by a sum of Slater-type orbitals

$$P_{nl}(r) = \sum_j C_{jnl} r^{I_{jnl}} \exp(-\xi_{jnl} r). \qquad (2)$$

The parameters ξ_{jnl} and coefficients C_{jnl} are determined by a variational optimization of the energy of a particular state, whilst the powers of $r(I_{jnl})$ remain fixed.

Table 1. Calculated energies (in Ry) for the target Be-like ions relative to the ground state compared with the NIST[11] values.

	N^{3+}		O^{4+}		F^{5+}	
level	NIST	present	NIST	present	NIST	present
$2s^2\ ^1S$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$2s2p\ ^3P^o$	0.6137	0.6136	0.7494	0.7491	0.8852	0.8787
$^1P^o$	1.1910	1.2100	1.4471	1.4698	1.7027	1.7106
$2p^2\ ^3P$	1.6008	1.6012	1.9478	1.9535	2.2953	2.2844
^1D	1.7212	1.7340	2.1116	2.1289	2.5024	2.5023
^1S	2.1448	2.1804	2.6236	2.6625	3.1023	3.1143
$2s3s\ ^3S$	3.4381	3.4584	4.9844	4.9753	6.8098	6.8058
^1S	3.5435	3.5464	5.1147	5.1110	6.9657	6.9568
$2s3p\ ^1P^o$	3.6863	3.6997	5.2929	5.2884	7.1794	7.1732
$^3P^o$	3.6998	3.7011	5.3116	5.3037	7.2025	7.1901
$2s3d\ ^3D$	3.8278	3.8411	5.4746	5.4769	7.4011	7.4018
^1D	3.9108	3.9369	5.5826	5.5986	7.5348	7.5488
$E_{IP}(2s^22p\ ^2P^o)$	3.4875	3.4728	5.6898	5.6713	8.3967	8.3795
$E_{IP}(2s2p^2\ ^4P)$	2.9655	2.9588	5.0369	5.0269	7.6113	7.6106

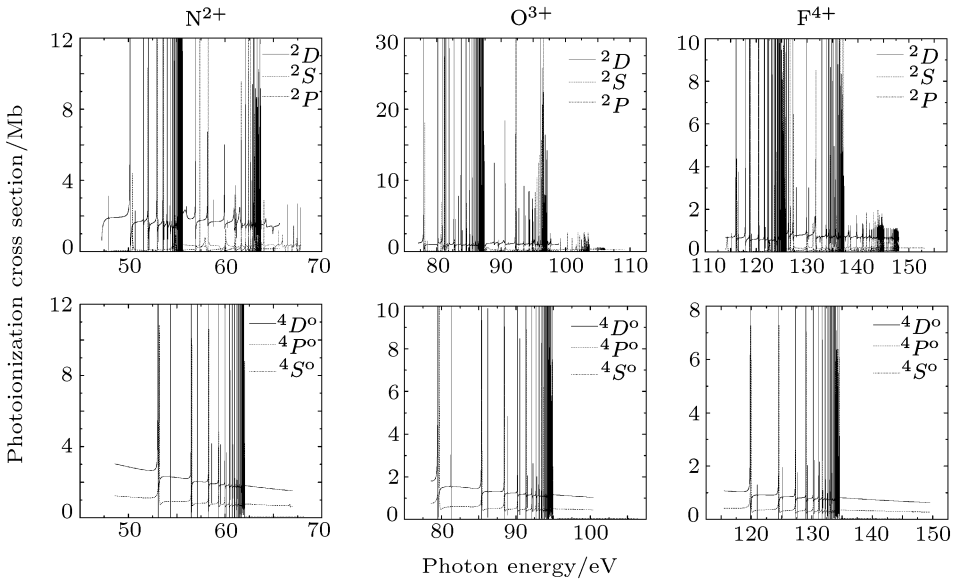


Fig.1. The photoionization cross sections as a function of the photon energy (eV) for B-like ions N^{2+} (left), O^{3+} (centre) and F^{4+} (right). Top: for the ground state $2s^22p\ ^2P^o$; bottom: for the excited state $2s2p^2\ ^4P$.

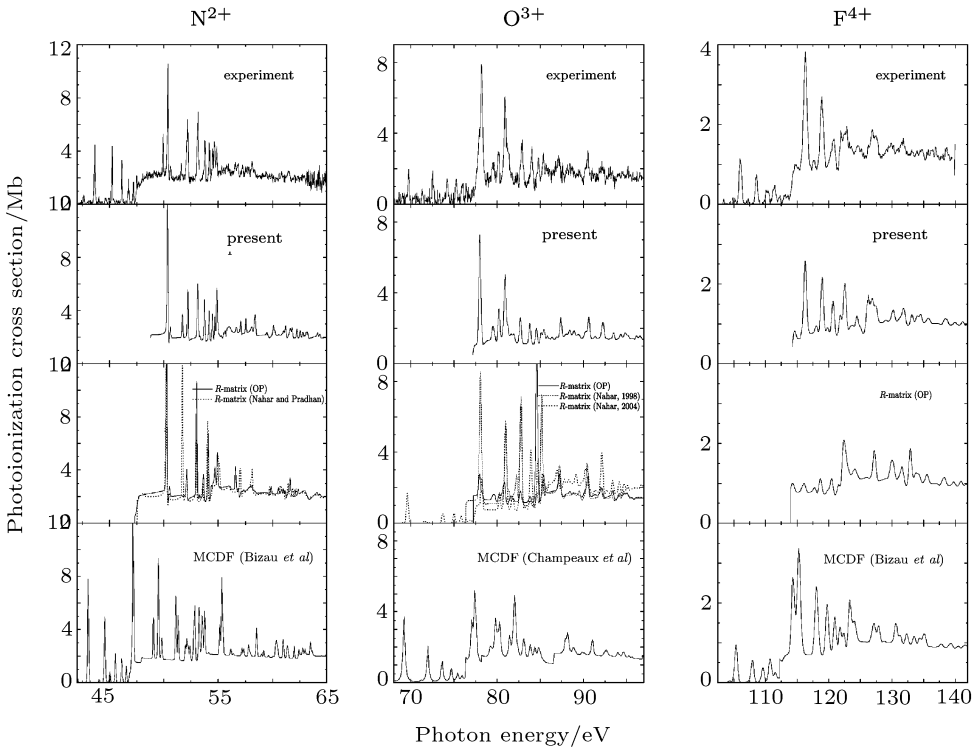


Fig.2. Comparison among different results for the photoionization cross sections of ions N^{2+} (left), O^{3+} (centre), F^{4+} (right). Top: the experimental data of Bizau *et al*;[8] Second: present *R*-matrix calculations; Third: previous *R*-matrix calculations from OP[2] and Nahar and Pradhan[3] for N^{2+}, OP[2] and Nahar[4,5] for O^{3+}, OP[2] for F^{4+}; bottom: the MCDF calculations from Bizau *et al* [8] and Champeaux *et al.*[7] The theoretical spectra are convoluted with Gaussian distributions of 100, 250 and 500 meV (FWHM), respectively, and are calculated under the assumption of a ($^2P^o$:^4P) fraction of (0.90:0.10) for N^{2+} and F^{4+} and (0.84:0.16) for O^{3+}. For N^{2+} and F^{4+}, we have shifted calculated energy scale by about 0.15, 0.25 eV, respectively, to the higher-energy side for ground state.

3. Results and discussions

In our calculations we include twelve lowest target states which are listed in Table 1, in which the energy levels we calculated are compared with those from experiments.[11] In the wave-function expansion of these target ions, six real and three pseudo-orbitals (1s, 2s, 2p, 3s, 3p, 3d, $\overline{4s}$, $\overline{4p}$, $\overline{4d}$) are included. The 1s, 2s and 2p orbitals are Hartree–Fock orbitals for the Be-like ground state $1s^22s^2\ ^1S$ given by Clementi and Roetti.[12] The pertinent parameters and coefficients for other orbitals are obtained by optimizing given energy of states using the CIV3 code.[13] The calculated energies for target states and ionization energies accord very well with experimental values. We employ a fine energy mesh of $10^{-6} \times z^2$ Ry, $z = Z - N$, where Z is the charge on the nucleus and N is the number of electrons included in the target.

Figure 1 displays calculated partial photoionization cross sections of N^{2+}, O^{3+} and F^{4+}, for ground state $2s^22p\ ^2P^o$ and excited state $2s2p^2\ ^4P$. In the near threshold range, the allowed one-electron transitions are $2s^22p\ ^2P^o + h\nu \rightarrow 2s^2(^1S)ns\ ^2S$, $nd\ ^2D$ and $2s2p^2\ ^4P + h\nu \rightarrow 2s2p(^3P)ns\ ^4P^o$, $nd\ ^4P^o$, $^4D^o$ under *LS*-coupling. Figure 2 displays a comparison between experimental and theoretical results. Our calculated results are convoluted with 100, 250 and 500 meV and summed with mixing fractions 90%, 84% and 90% for $^2P^o$, 10%, 16% and 10% for ^4P in the case of N^{2+}, O^{3+} and F^{4+}, respectively. In Fig.3 we give a more detailed comparison between the present and experimental results of Bizau *et al.*[8] For N^{2+} and F^{4+}, we have shifted calculated energy scale by about 0.15 and 0.25 eV, respectively, toward the higher-energy side for the ground state. It can be observed from Figs.2 and 3 that some resonances observed in experiment disappear in the *LS* coupling results. The missed resonances lie in the energy range $E(2s^2\ ^1S)$–$E(2s2p\ ^3P^o)$ for metastable state ^4P, they can be formed in this range from allowed transitions with relativistic fine structure, but not via *LS* coupling, $^4P_{1/2,3/2,5/2} + h\nu \rightarrow 2s^2(^1S)np\ ^2P^o_{1/2,3/2}$. For N^{2+},

we also point out that the peak No.9 is also missed in all R-matrix calculations. Bizau *et al* [8] thought that this resonance was from the transition $2s^22p\ ^2P^o \rightarrow 2s2p(^3P)5p\ ^2P$. However, the ^2P term cannot autoionize into the $1s^22s^2\ ^1S+\epsilon p$ continuum and its presence must be due to autoionization through relativistic effects. In the present paper, we focus on the photoionizations which can be produced in LS calculations in which the relativistic effect is not taken into consideration.

The photoionization cross sections of the B-like ions N^{2+}, O^{3+} and F^{4+} have been calculated utilizing the R-matrix method by Fernley *et al* [2] as part of the Opacity Project. In their calculation, Fernley *et al* included six target states in configurations $1s^22s^2$, $1s^22s2p$ and $1s^22p^2$. Employing the same method, Nahar and Pradhan[3] calculated the cross sections of the ions of C and N (for N^{2+} ion they included 12 target states). Nahar[4] calculated the cross sections for oxygen and its ions (a 12-CC eigenfunction expansion is used). All the above investigations were non-relativistic and R-matrix calculations including relativistic effects have been carried out for oxygen ions by Nahar[5] (for O^{3+}, the target eigenfunctions consist of a 20-level expansion). These results are also shown in Fig.2 (third panels) and we can see that these calculations are able to reproduce the magnitude of the continuum cross sections, but fail to describe many details of the spectral structures, especially for O^{3+} and F^{4+}. And for O^{3+}, the peak No.8 was missing in the Nahar's calculations.

Using the MCDF method Bizau *et al* [8] and Champeaux *et al* [7] calculated photoionization cross sections for N^{2+}, F^{4+} and O^{3+}, respectively. And the results are displayed in Fig.2 (bottom panels). The MCDF description of the cross sections is fairly good for the gross features but fails to give resonance positions correctly. As can be seen later, the peaks are shifted in energy by up to ±1 eV.

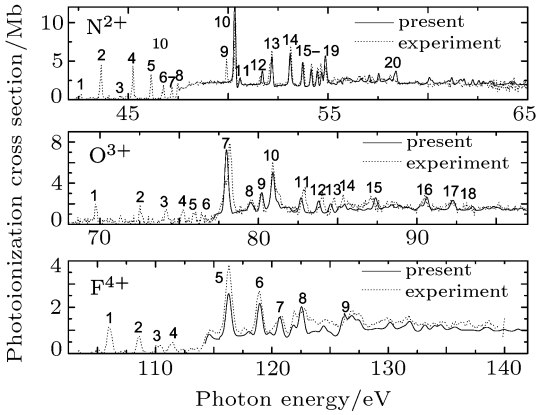


Fig.3. Comparison of photoionization cross sections as a function of photon energy (eV) between present R-matrix calculations and measurements by Bizau *et al* [8] for N^{2+} (top), O^{3+} (middle), F^{4+} (bottom). For N^{2+} and F^{4+}, we have shifted the calculated energy scale by about 0.15, 0.25 eV, respectively, toward the higher-energy side for ground state.

From Figs.2 and 3 we can see that the present calculations show a significant improvement over the previous theoretical results. The magnitudes of the continuum cross sections, spectral structures and peak positions are in good agreement with the recent experimental results of Bizau *et al.*[8]

Table 2. Locations and designations of the resonances in the photoionization spectrum of N^{2+}. The peak numbers refer to those in Fig.3. The experimental and MCDF results are cited from Ref.[8]. The NIST and MCDF values are in accordance with assignments given by Bizau *et al.*[8]

	resonance energy/eV				final state	
peak	exp.	NIST	MCDF	present	Bizau *et al*	present
10	50.37	50.37	49.48	50.18	$2s2p(^3P)5p\ ^2D$	$2s2p(^3P)5p\ ^2D$
11	50.61	50.61	49.81	50.44	$2s2p(^3P)5p\ ^2S$	$2s2p(^3P)5p\ ^2S$
12	51.61	51.54		51.56	$2p^2(^3P)3d\ ^2D$	
13	52.19	52.10	51.33	52.04	$2s2p(^3P)6p\ ^2P$	$2s2p(^3P)6p\ ^2D,^2S$
		52.21	51.11		$2s2p(^3P)6p\ ^2D$	
14	53.14	53.13	52.11	52.96	$2s2p(^3P)7p\ ^2P,^2D$	$2s2p(^3P)7p\ ^2D,^2S$, $2p^2(^3P)4p\ ^4D^o,^4P^o$
15	53.77	53.75	52.86	53.58	$2s2p(^3P)8p\ ^2P,^2D$	$2s2p(^3P)8p\ ^2D,^2S$
16	54.18	54.20	53.24	54.01	$2s2p(^3P)9p\ ^2P,^2D$	$2s2p(^3P)9p\ ^2D,^2S$
17	54.49	54.51	53.53	54.32	$2s2p(^3P)10p\ ^2P,^2D$	
18	54.65	54.66	55.14	54.54	$2s2p(^1P)4p\ ^2D$	
19	54.86	54.85	55.32	54.70	$2s2p(^1P)4p\ ^2P$	
20	58.13	58.15	58.54	58.18	$2s2p(^1P)5p\ ^2P,^2D$	$2s2p(^1P)5p\ ^2D$
				58.25		$2s2p(^1P)5p\ ^2P$

Although the R-matrix approach cannot be used to identify the peaks straightforwardly, the partial cross sections can still provide some useful information. In Fig.4 we display the partial cross sections and for the sake of clarity the convoluted results are given. The assignments of peaks together with the measured and calculated energies are given in Tables 2–5. Firstly, from the top panel in Fig.4 and Table 2 for N^{2+}, we can see that the difference in assignment between the present and Bizau *et al*'s [8] results is that the ^2P symmetry is absent in our calculations while the ^2S symmetry is absent in their results. Bizau *et al* identified the peak No.12 from NIST as the $2p^2(^3P)3d\ ^2D$. It should be pointed out that we cannot find $2p^2(^3P)3d\ ^2D$ state in the updated NIST Atomic Spectra Database Version 3.1.2. Beside the resonances coming from ground state there are also some strong peaks due to transitions from metastable states. The peak No.14 is not only from ground state but also from metastable state. We identify these resonances from NIST as $2p^2(^3P)np\ ^4D^o,^4P^o$ transition from the metastable state and compare with their energies in Table 3. We can see that the present results are in good agreement with NIST values, the difference between them is less than 0.1 eV. Bizau *et al* pointed out that the assignment of peaks labeled as 17–19 was difficult since there was to some degree the configuration interaction between the $2s2p(^3P)(n\geq 10)p\ ^2D$, ^2P, ^2S and the corresponding $2s2p(^1P)4p$ terms. We are not sure exactly whether these resonances should be identified.

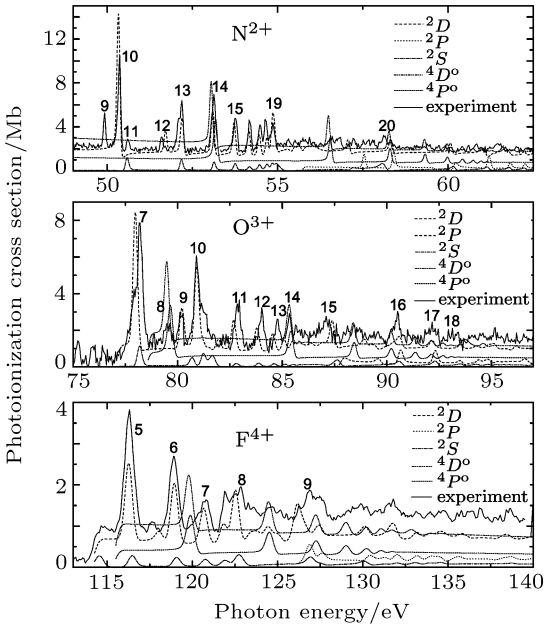


Fig.4. Photoionization cross sections of N^{2+} (top), O^{3+} (middle), F^{4+} (bottom). The theoretical spectra are convoluted with experimental bandwidth.

Table 3. Energies of the resonances $2p^2(^3P)np\ ^4D^o,^4P^o$ (in eV) for N^{2+}, O^{3+} and F^{4+}. Values are compared, where available, to values from the NIST[11] and Ref.[14].

	N^{2+}		O^{3+}			F^{4+}
level	NIST	present	NIST	[14]	present	present
$2p^2(^3P)4p\ ^4D^o$	53.11	53.05	79.52	79.38	79.46	120.79
$^4P^o$	53.25	53.19			79.65	120.88
$2p^2(^3P)5p\ ^4D^o$	56.57	56.49			85.33	125.47
$^4P^o$	56.63	56.54			85.41	125.52
$2p^2(^3P)6p\ ^4D^o$	58.36	58.27			88.40	128.24
$^4P^o$	58.39	58.30			88.44	128.26
$2p^2(^3P)7p\ ^4D^o$	59.41	59.31			90.20	130.01
$^4P^o$	59.42	59.33			90.22	130.02

Now, we turn our attention to the peak No.8 in the spectrum of O^{3+} (middle panel in Fig.3). Champeaux *et al* [7] assigned this peak to the transition from the ground state to the ^2S term of the $2s2p(^3P)5p$ configuration, but it would imply a very large splitting between the ^2S and ^2D terms and Bizau *et al* did not give designation for this peak. It can be easily seen from Fig.4 that this peak is due to transition from metstable state and we assign the peak No.8 as $2p^2(^3P)4p\ ^4D^o,^4P^o$ according to the case of N^{2+}. In Table 3 we also list the energies of $2p^2(^3P)np\ ^4D^o,^4P^o(n=4–7)$ for O^{3+} and F^{4+}. Around the peak No.10 there are several resonances but the main contribution comes from $2s2p(^3P)6p\ ^2D$. From Fig.4 we can see that the peak No.14 is due to overlapping transitions from ground state to $2s2p(^3P)10p\ ^2D$, ^2S and from metstable state to $2p^2(^3P)5p\ ^4D^o$, $^4P^o$, so it is stronger than the peak No.13.

Table 4. Locations and designations of the resonances in the photoionization spectrum of O^{3+}. The peak numbers refer to those in Fig.3. The experimental and MCDF results are cited from Ref.[8]. The NIST and MCDF values are in accordance with assignments given by Bizau *et al.*[8]

	resonance energy/eV				final state	
peak	exp.	NIST	MCDF	present	Bizau *et al*	present
7	78.16	78.3	77.4	77.98	2s2p(^3P)5p ^2P, ^2D, ^2S	2s2p(^3P)5p ^2D, ^2S
8	79.53			79.51		2p^2(^3P)4p $^4D^o$, $^4P^o$
9	80.16	80.20	79.82	80.21	2p^2(^3P)3d ^2D	2p^2(^3P)3d ^2D
10	80.9		80.2	80.91	2s2p(^3P)6p ^2P, ^2D, ^2S	2s2p(^3P)6p ^2D
		81.43	82.3		2s2p(^1P)4p ^2P, ^2D, ^2S	
11	82.88		81.9	82.69	2s2p(^3P)7p ^2P, ^2D	2s2p(^3P)7p ^2D, ^2S
12	84.01		83.12	83.80	2s2p(^3P)8p ^2P, ^2D	2s2p(^3P)8p ^2D, ^2S
13	84.78		83.84	84.56	2s2p(^3P)9p ^2P, ^2D	2s2p(^3P)9p ^2D, ^2S
14	85.35		84.37	85.43	2s2p(^3P)10p ^2P, ^2D	2s2p(^3P)10p ^2D, ^2S, 2p^2(^3P)5p $^4D^o$, $^4P^o$
15	87.11		88.15	87.38	2s2p(^1P)5p ^2P, ^2D	2s2p(^1P)5p ^2D
16	90.47		91.09	90.63	2s2p(^1P)6p ^2P, ^2D	2s2p(^1P)6p ^2P, ^2D
17	92.14		92.8	92.28	2s2p(^1P)7p ^2P, ^2D	2s2p(^1P)7p ^2P, ^2D
18	93.15		93.99	93.52	2s2p(^1P)8p ^2P, ^2D	2s2p(^1P)8p ^2P, ^2D

Table 5. Locations and designations of the resonances in the photoionization spectrum of F^{4+}. The peak numbers refer to those in Fig.3. The experimental and MCDF results are cited from Ref.[8].

	resonance energy/eV			final state	
peak	exp.	MCDF	present	Bizau *et al*	present
5	116.31	115.4	116.03	2s2p(^3P)6p ^2P, ^2D, ^2S	2s2p(^3P)6p ^2D, ^2S
6	118.97	117.9	118.71	2s2p(^3P)7p ^2P, ^2D	2s2p(^3P)7p ^2D, ^2S
7	120.83	118.7	120.43	2s2p(^3P)8p ^2P, ^2D	2s2p(^3P)8p ^2D, ^2S
8	122.7	123.3	122.30	2s2p(^1P)5p ^2P, ^2D	2s2p(^3P)9p ^2D, ^2S
				2s2p(^3P)($n\geq 9$)p	2s2p(^1P)5p ^2D, ^2S
9	127.1	127.9	126.60	2s2p(^1P)6p ^2P, ^2D	2s2p(^1P)6p ^2D, ^2P, ^2S

4. Conclusion

We calculate photoionization cross sections of B-like ions N^{2+}, O^{3+} and F^{4+} which are in excellent agreement with the recent measurements. In the present calculations we also find the resonances 2p^2(^3P)np $^4D^o$,$^4P^o$. Our results show a good improvement over the previous theoretical results. For excited states of these ions we still need a relativistic calculation in comparison with the available experimental results.

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