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ENERGY SPECTRA OF THE TUNGSTEN ION $4s^24p^N$, $4s^24p^{N-1}4d$ AND $4s4p^{N+1}$ CONFIGURATIONS

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The *ab initio* quasirelativistic Hartree–Fock approximation was used to determine spectroscopic parameters for the multicharged tungsten ions with an open 4p shell. The configuration interaction method based on the transformed radial orbitals was applied to include the electron-correlation effects. The relativistic effects were taken into account in the Breit–Pauli approximation for the quasirelativistic Hartree–Fock radial orbitals. The complete energy level spectra were calculated for the $4s^24p^N$, $4s^24p^{N-1}4d$ and $4s4p^{N+1}$ configurations of the tungsten ions from W^{43+} to W^{38+}.

Keywords: quasirelativistic approach, many-electron ions, energy levels, tungsten

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1. Introduction

Owing to its unique physical features, metallic tungsten is widely utilized in various high-temperature devices, including fusion reactors [1, 2]. Even if tungsten resists vaporization, highly-charged ions of tungsten can emerge in fusion plasma and decrease its temperature.

A wide compilation of the spectroscopic data for the tungsten ions was published [3], where the semiempirical data were also included. Later those data were supplemented in [4]. Although the energy spectra of the configurations with open 4p shells are quite simple, the experimental data are usually known only for few levels of the ground configuration and for some levels of excited configurations. Even if the theoretical and the experimental studies of the tungsten ions are important in fusion plasma research, both the experimental and the theoretical spectroscopic data for the ions from W^{38+} to W^{43+}, i. e. the ions with the ground configuration $4s^24p^N$, are scarce. Just few ions are investigated theoretically in more detail. The investigation of the W^{39+} ion radiative transition properties is discussed in [5], where the energy level spectra of the Br-like tungsten ion with the ground configuration $4s^24p^5$ are determined using the quasirelativistic approach. This ion is also included in the present investigation as we want to study consistently the entire set of the tungsten ions with the ground configurations $4s^24p^N$.

The theoretical investigation of several excited configurations of various tungsten ions is presented in [6]. The calculations are performed applying a fully-relativistic parametric-potential code RELAC [7]. Unfortunately, the results for the energy levels in [6] are incomplete – quite a large number of the excited state levels is missing.

The fully relativistic multiconfiguration Dirac–Fock (MCDF) approach is applied to determine the energy levels of the ground configurations for the ions from W^{29+} to W^{42+} in [8]. The magnetic dipole (M1) and electric quadrupole (E2) transition probabilities among the levels of the ground configurations are also calculated.

The W^{43+} ion with only one electron in the 4p shell was investigated using various theoretical approaches [9–12]. The ion W^{42+} was also investigated in [12]. Unfortunately, most of these studies do no present complete energy level spectra for the lowest to excited configurations – usually, data for one or more of the excited configuration levels are missing. In the present work we study the tungsten ions with an open 4p shell, i. e. ions from W^{38+} to W^{43+}. The ground configuration $4s^24p^N$ and two excited configurations $4s^24p^{N-1}4d$ and $4s4p^{N+1}$ are investigated. These excited configurations are investigated as a unified system as they are energetically very close. The main goal of the present study is to determine complete and as accurate as possible energy level spectra of the tungsten ion configurations under study.

In Section 2 we provide a short description of the adopted calculation method. Since this approximation completely matches the one applied for

the tungsten investigation in [13–16], here we provide only a brief summary of our quasirelativistic approach. The calculation results are discussed and compared with the results of other authors in Section 3. The summary and the main conclusions are presented in Section 4.

2. Calculation method

Similarly to our previous investigations, we perform the calculations using the solutions of the quasirelativistic Hartree–Fock equations [17–19]. The details of the quasirelativistic approximation are decribed in more detail in [20]. A brief description of our quasirelativistic method is given in [14, 15].

The radial orbitals (RO) describing the electrons of the configurations under study (adjusted configurations) are determined by solving the quasirelativistic Hartree–Fock equations (QRHF) [18, 19] for the ground configuration. The quasirelativistic RO of 4d electron and 4f electron are calculated using the frozen-core potential for the $4p^{N-1}nl$ configuration. The virtually excited electrons with $n > 4$ are decribed by the quasirelativistic transformed radial orbitals (TRO) [20]. Like in the previous investigations of tungsten ions [13–16], the variable parameters of TRO are determined by ensuring the maximum value of the correlation correction. TRO are determined for the radial orbitals with the principal quantum number $5 \le n \le 10$ and with all possible values of the orbital quantum number l.

This set of RO is used for both the even and the odd configurations. By applying such an approximation, we are able to avoid the problems of non-orthogonality in the calculation of the radiative transition parameters and the electron-impact excitation data. Therefore we must include more configurations in the CI wavefunction expansion in order to determine accurate energy level eigenvalues and eigenfunctions. For the calculation of the level energies, the one-electron and the two-electron relativistic corrections are included in the Breit–Pauli approximation. Their adoption for the quasirelativistic approach is described in [20].

The correlation corrections are included by applying the configuration interaction (CI) method. The CI wavefunction expansion is based on the set of the admixed configurations that are produced by promoting one or two electrons from the $3l$ and $4l$ shells of the adjusted configurations to all states possible in the generated RO basis.

This large basis of determined radial orbitals allows us to construct a large number of the admixed configurations, and consequently to include various types of the correlation effects, including the core-polarization correction. The total number M of possible admixed configurations is very large due to a large basis of TRO. Nevertheless, some of these generated admixed configurations are not important when the level energies of the adjusted configurations are calculated. So further selection of the admixed configurations is performed employing the average weights $\bar{w}_{PT}$ of the admixed configurations. These weights are determined in the second order of the many-body perturbation theory [21]. If $\bar{w}_{PT}$ of the particular admixed configuration is larger than the arbitrary selection criterion w_{min}, then that configuration is included into the CI wavefunction expansion. The selection criteria applied here for the investigated ions are smaller than 1×10^{-6} in the present work.

The majority of the admixed configurations have several open shells. Therefore, the number of generated LS-coupling terms, the so-called configuration state functions (CSF), is very large. The total number of CSF is reduced by moving the shells with the virtual excited electrons to the beginning of the list of the active shells and by excluding the CSF terms that do not interact with the adjusted configuration. This reduction technique is fully described in [22]. Furthermore, the correlation corrections are accounted in full after this reduction procedure, even if the Hamiltonian matrix order becomes significantly smaller.

Table 1 presents the exact numbers M of generated admixed configurations and the numbers S of the selected ones for the ground configuration and for the complex of excited configurations. The index "g" denotes the calculation parameters of the ground configurations, the index "e" denotes the calculation parameters of the complex of the excited configurations. There are also the total numbers C of CSF and the numbers R of CSF after the reduction. The data are presented for each investigated ion. From this table one can see clearly that the investigation of the excited configurations is more complicated than the study of the ground configuration. The applied methods of the selection of the admixed configurations and the CSF reduction very effectively simplify the calculations. Finally, the determined sets with R_e and R_g of CSF are employed to compute the level energies of the tungsten ions.

To perform our calculations, we have employed our own original computer codes together with the codes [23–25] that have been adapted for our computing needs. The code from [23] was updated according to the methods presented in [26, 27].

3. Results and discussion

Our calculated level energies are presented in the following tables and are compared with the experimental

Table 1. Calculation parameters for the ground configurations and for two excited configurations.

	W^{43+}	W^{42+}	W^{41+}	W^{40+}	W^{39+}	W^{38+}
M_g	3440	3490	3490	3490	3222	3139
S_g	244	420	284	324	191	201
C_g	163947	876758	511156	1039490	122078	38023
R_g	2816	20496	19743	24848	2992	749
M_e	7084	8005	8005	8005	7286	4574
S_e	1366	1866	830	900	961	880
C_e	3077206	9054212	5477512	7199922	612207	4271190
R_e	95463	439491	395428	539211	432564	119568

data from compilation [28], further named as "NIST" and with available theoretical calculations by other authors. The semiempirical data from the NIST collection are placed in the square brackets. All our data tables present the number (index) of level (the levels are numbered according to their QR energy ascending order), CSF in the *LS*-coupling notation and the total angular momentum *J*. Our computer code assigns the level to one or another *LS* term according to their maximum weight in the eigenfunction determined after the diagonalization of the Hamiltonian matrix. This can lead to the situation when several levels with the same *J* can be prescribed with the same *LS* term. We add a supplementary index "a" to the levels with the same *LSJ*. Along with the level energies we determine the relative deviations Δ from the NIST data:

$$\Delta = \frac{E^{\text{th}} - E^{[28]}}{E^{[28]}} \times 100\%.$$

In all level energy data tables for the W^{43+}–W^{38+} ions, we present the comparison of our QR results with the NIST data [28]. Furthermore, the relativistic calculation results from [6], marked as "RELAC" [6], and the theoretical data from the MCDF calculation [8] are given in Tables 2–7. These tables also contain the results of other authors if such data are available. Table 2 contains only the RELAC [6] data as the ion W^{38+} has only one level in the ground configuration $4p^6$. There is no point to present the MCDF [8] results in Tables 2 and 6 as the ground configuration of the ions W^{43+} and W^{39+} has only two levels.

3.1. W^{43+} *energy levels*

The ground configuration of the gallium-like tungsten is $4s^24p$. All three investigated configurations $4s^24p$, $4s^24d$ and $4s4p^2$ have twelve energy levels. The NIST database provides eight level energies, and the energy for one of them is determined from the semiempirical calculations. Our calculated data are presented in Table 2. Here we also tabulate the data from [28] and the theoretical results from [6, 9–12]. According to the MCDF results from [8], the energy of the level $4s^24p\ ^2P_{3/2}$ is equal to 790710 cm^{-1} and Δ = –0.14%. The agreement between our results and the experimental NIST data is

Table 2. The level energies *E* (in 100 cm^{-1}) of the W^{43+} ion and their relative deviations Δ (in %) from the NIST [28] data.

N	CSF	*J*	NIST	QR		RELAC [6]		MCDF [9]		MCDF [10]		MCDHF [11]		FAC [12]	
			E	*E*	Δ	*E*	Δ	*E*	Δ	*E*	Δ	*E*	Δ	*E*	Δ
1	$4s^24p\ ^2P$	0.5	0	0		0		0		0		0		0	
2	$4s4p^2\ ^4P$	0.5	7802	7808	0.07	7870	0.87	7856	0.68	7806	0.05	7802	0.00	7798	–0.06
3	$4s^24p\ ^2P$	1.5	7918	7915	–0.04	7936	0.23	7909	–0.11	7916	–0.03	7916	–0.02	7915	–0.05
4	$4s4p^2\ ^4P$	1.5	[14660]	14649	–0.08	14626	–0.23	14659	0.00	14638	–0.15	14653	–0.04	14616	–0.30
5	$4s4p^2\ ^2D$	2.5	15336	15328	–0.05	15368	0.21	15361	0.16	15336	0.00	15337	0.00	15315	–0.14
6	$4s4p^2\ ^2D$	1.5	16304	16318	0.08	16442	0.85	16364	0.37	16312	0.05	16308	0.02	16314	0.06
7	$4s4p^2\ ^2P$	0.5	16497	16515	0.11	16701	1.23	16611	0.69	16513	0.09	16505	0.05	16557	0.36
8	$4s^24d\ ^2D$	1.5	20876	20847	–0.14	20992	0.56	20958	0.40					20928	0.25
9	$4s^24d\ ^2D$	2.5		22033		22088		22073						22047	
10	$4s4p^2\ ^4P$	2.5		23464		23568		23547				23539			
11	$4s4p^2\ ^2S$	0.5		24420				24502				24435		24441	
12	$4s4p^2\ ^2P$	1.5		24721				24831				24729		24781	

fine. The largest disagreement appears for the level 8 energy. Even in this case the relative deviation $\Delta = -0.14\%$ is rather small. It looks favourable when compared to the data from other sources [6, 9], whereas the data for this level are missing in [10, 11]. The deviations are even smaller for other levels. Therefore we assume that the level energies for the next four higher levels have similar accuracy.

3.2. W^{42+} *energy levels*

The investigated configurations $4s^24p^2$, $4s^24p4d$ and $4s4p^3$ of the germanium-like tungsten ion are coupled into 27 *LSJ* levels. The NIST database tabulates energies of ten levels, although two values are determined from the semiempirical calculations [3]. Our determined results are presented in Table 3. One can see from Table 3 that our QR results are in good agreement with the experimental data. The largest deviation Δ appears for the level $4s^24p^2\ ^3P_1$ ($N = 2$). For other levels, Δ is significantly smaller than 0.5%. The Δ values in Table 3 indicate that our QR results are more accurate than the data from [6] and have very similar accuracy to that of the relativistic MCDF results [8]. The comparison with the FAC calculation data from [12] points out that our QR calculation data are slightly less accurate for four levels (out of six) given there. Probably, it is important to note that only four levels of excited configurations (out of 22 levels) are presented in [12].

Table 3. The level energies E (in 100 cm^{-1}) of the W^{42+} ion and their relative deviations Δ (in %) from the NIST [28] data.

N	CSF	J	NIST	QR		RELAC [6]		MCDF [8]		FAC [12]	
			E	E	Δ	E	Δ	E	Δ	E	Δ
1	$4s^24p^2\ ^3P$	0	0	0		0		0		0	
2	$4s^24p^2\ ^3P$	1	7383	7336	–0.64	7296	–1.17	7361	–0.30	7373	–0.13
3	$4s^24p^2\ ^1D$	2	7727	7722	–0.07	7659	–0.89	7772	0.57	7728	0.00
4	$4s4p^3\ (^2P)\ ^3P$	2	15138	15152	0.10	15146	0.05			15114	–0.16
5	$4s^24p^2\ ^3P$	2	[15350]	15364	0.09	15347	–0.02	15347	–0.02		
6	$4s^24p^2\ ^1S$	0	[16090]	16130	0.25	16123	0.21	16123	0.21		
7	$4s4p^3\ (^2D)\ ^3D$	1	16312	16372	0.37	16442	0.80			16346	0.20
8	$4s^24p4d\ ^3F$	2	19734	19800	0.34	19745	0.06			19715	–0.09
9	$4s^24p4d\ ^3D$	1	21191	21235	0.21	21365	0.82			21273	0.39
10	$4s4p^3\ (^4S)\ ^5S$	2		21594						21536	
11	$4s^24p4d\ ^3F$	3		21950		21950				21911	
12	$4s4p^3\ (^2D)\ ^3D$	2		22915							
13	$4s4p^3\ (^2D)\ ^3D$	3		23276							
14	$4s4p^3\ (^2P)\ ^3P$	0		23546							
15	$4s4p^3\ (^2P)\ ^3P$	1		24104						24055	
16	$4s4p^3\ (^2D)\ ^1D$	2		24326		24426					
17	$4s4p^3\ (^4S)\ ^3S$	1		24437						24440	
18	$4s^24p4d\ ^3D$	2		28465							
19	$4s^24p4d\ ^3P$	1		28567							
20	$4s^24p4d\ ^3P$	0		28627							
21	$4s^24p4d\ ^3F_a$	3		28662							
22	$4s^24p4d\ ^3F$	4		29281							
23	$4s^24p4d\ ^3P$	2		29334							
24	$4s^24p4d\ ^3D$	3		30819							
25	$4s^24p4d\ ^1P$	1		30921							
26	$4s4p^3\ (^2P)\ ^3P_a$	2		31755							
27	$4s4p^3\ (^2P)\ ^1P$	1		32798							

3.3. W^{41+} *energy levels*

The ground configuration of the arsenic-like tungsten ion $4s^24p^3$ and its excited configurations $4s^24p^24d$ and $4s4p^4$ produce 41 levels. Twelve level energies are presented in the NIST database, nevertheless, the energies of two levels are coming from the semiempirical study [3]. These data together with the QR results are presented in Table 4. In the process of the comparison of our QR results with the NIST data, the level $4s4p^4$ (^{3}P) $^4P_{5/2}$ (N = 6) stands out. In the NIST database, this level is assigned to the configuration $4s^24p^24d$. As mentioned earlier in this section, our computer code assigns the level to one or another *LS* term according to their maximum weight within the level eigenfunction. The level N = 6 is identified as the $4s4p^4(^3P)^4P$, and its maximum weight equals to 27%. A more detailed analysis of the eigenfunction indicates that the term $4s^24p^2(^4S)4d\ ^5D$ with the weight value of 26% makes the second largest by weight contribution. The sum of the weights of the terms assigned to the $4s^24p^24d$ in this eigenfunction is close to 70%. Hence the level N = 6 must be assigned to the $4s^24p^24d$ configuration instead of the configuration $4s4p^4$, even if its *LS* term has the maximum weight. A similar situation occurs for the levels N = 17 and N = 26. The discussed wavefunction expansion of the terms confirms the fact that the excited configurations $4s4p^4$ and $4s^24p^24d$ mix very strongly. Therefore they must be studied together instead of being investigated separately.

The agreement between our QR results and the NIST data for this ion is slightly worse compared to the ions W^{42+} and W^{43+}. The results [6] calculated employing the parametric potential are not highly accurate either as it is evident from the values of the relative deviations Δ. The comparison of our QR results and those from the MCDF approach [8] for the ground configuration indicates that the accuracy of both methods is similar. All available theoretical results significantly differ from the level energies determined by the semiempirical calculation for the level N = 4.

3.4. W^{40+} *energy levels*

The ground configuration of the selenium-like tungsten is $4s^24p^4$. This configuration and two excited configurations $4s^24p^34d$ and $4s4p^5$ form 47 energy levels. The NIST database contains data for thirteen energy levels. One of them is determined by the semiempirical calculation [3].

Similar to the previous data tables, Table 5 presents our QR results, the NIST data and two theoretical calculations, namely RELAC and MCDF. The agreement with experiment of the QR results is slightly worse compared to the MCDF [8] results. The large difference between the experimental data and the RELAC results for the level N = 2 energy is very uncommon for the data from calculation [6]. For the highly excited levels of the $4s4p^5$ configuration, the agreement with the experimental data is better for the QR results than for the RELAC calculations. The accuracy of the QR results for some levels of the $4s^24p^34d$ configuration (N = 18, 19, 21) is noticeably worse. This is also the case for the RELAC data.

The level N = 9 is assigned to the configuration $4s4p^5$ according to the maximum weight of term in the CI wavefunction expansion, but the sum of the other term weights confirms that it must be assigned to the configuration $4s^24p^34d$. A similar case was discussed for the level N = 6 of the W^{41+} ion. The levels N = 11 and N = 12 in our calculation have their position swapped around compared to the NIST data, but the difference of these level energies is tiny. Furthermore, the energy of the level N = 11 in the NIST database is derived from the semiempirical calculations [3] rather than the experiment.

3.5. W^{39+} *energy levels*

We investigate the spectroscopic parameters of the bromine-like tungsten ion. The earlier investigation of the radiative transitions for this ion is presented in [5]. The ground configuration $4s^24p^5$ and two excited configurations $4s^24p^44d$ and $4s4p^6$ produce 31 levels. The NIST database reports only 12 level energies for these configurations, all of them are determined from the experiment.

This ion draws more attention than other tungsten ones discussed in the present study. The reported investigation of W^{39+} is not limited to previously discussed studies [6, 8]. The review of the MCDHF calculation methods is illustrated by the study of this ion in [29]. Moreover, the energy level spectra and the radiative transition parameters determined in the MCDF approximation were extensively discussed quite recently in [30, 31]. One can find more details on the subject of these works in [5]. This very recent work presents a comprehensive comparison of the QR data with the results of other theoretical investigations. Although the main purpose of the latter work was to study the radiative transition properties, the energy level spectra of the W^{39+} ion were also studied. The results presented in [5] slightly differ from the results of the present work as here all our calculations are performed in the same way for all tungsten ions with an open 4p shell, i. e. utilizing

Table 4. The level energies E (in 100 cm^{-1}) of the W^{41+} ion and their relative deviations Δ (in %) from the NIST [28] data.

N	CSF	J	NIST	QR		RELAC [6]		MCDF [8]	
			E	E	Δ	E	Δ	E	Δ
1	$4s^24p^3\ ^2P$	1.5	0	0		0		0	
2	$4s^24p^3\ ^4S$	1.5	7196	7138	−0.80	7091	−1.46	7160	−0.50
3	$4s^24p^3\ ^2D$	2.5	7621	7594	−0.36	7555	−0.87	7613	−0.10
4	$4s^24p^3\ ^2P$	0.5	[8020]	8175	1.93	8278	3.21	8187	2.09
5	$4s^24p^2(^3P)4d\ ^4F$	1.5	12363	12607	1.97	12496	1.07		
6	$4s4p^4(^3P)\ ^4P$	2.5	14255	14339	0.59	14327	0.51		
7	$4s^24p^3\ ^2P_a$	1.5	[15280]	15379	0.65			15426	0.96
8	$4s4p^4(^3P)\ ^4P_a$	2.5	15411	15479	0.44	15525	0.74		
9	$4s4p^4(^1S)\ ^2S$	0.5		16330		16453			
10	$4s4p^4(^3P)\ ^2P$	1.5	16467	16515	0.29	16643	1.07		
11	$4s^24p^2(3P)4d\ ^4F$	2.5		19725		19617			
12	$4s^24p^2(^3P)4d\ ^4F_a$	1.5	19573	19737	0.84				
13	$4s^24p^2(^3P)4d\ ^4D$	0.5		19761					
14	$4s^24p^2(^1D)4d\ ^2G$	3.5		20174		20079			
15	$4s^24p^2(^3P)4d\ ^4D$	3.5		21277		21226			
16	$4s^24p^2(^3P)4d\ ^4P$	2.5	21147	21298	0.71	21370	1.05		
17	$4s4p^4(^3P)\ ^4P$	1.5		21312		21326			
18	$4s^24p^2(^1D)4d\ ^2D$	1.5	21255	21391	0.64	21534	1.31		
19	$4s^24p^2(^3P)4d\ ^4P$	0.5		21460		21569			
20	$4s^24p^2(^1D)4d\ ^2D$	2.5		21638		21660			
21	$4s^24p^2(^1D)4d\ ^2G$	4.5		21774		21743			
22	$4s^24p^2(^1D)4d\ ^2F$	3.5		22884		22910			
23	$4s^24p^2(^3P)4d\ ^4P_a$	2.5		22898		22982			
24	$4s^24p^2(^3P)4d\ ^2D$	1.5		22916					
25	$4s^24p^2(^1D)4d\ ^2S$	0.5		23032		23118			
26	$4s4p^4(^3P)\ ^4P_a$	1.5		23379					
27	$4s4p^4(^1D)\ ^2D$	2.5		23818					
28	$4s4p^4(^3P)\ ^2P_a$	1.5		24611					
29	$4s4p^4(^3P)\ ^2P$	0.5		24644					
30	$4s^24p^2(^1D)4d\ ^2D_a$	1.5		28417					
31	$4s^24p^2(^3P)4d\ ^4P_a$	0.5		28447					
32	$4s^24p^2(^3P)4d\ ^4D$	2.5		28486					
33	$4s^24p^2(^3P)4d\ ^2F$	3.5		28673					
34	$4s^24p^2(^3P)4d\ ^2F_a$	3.5		29088					
35	$4s^24p^2(^3P)4d\ ^4F$	4.5		29162					
36	$4s^24p^2(^3P)4d\ ^2P$	0.5		29180					
37	$4s^24p^2(^1S)4d\ ^2D$	1.5		29349					
38	$4s^24p^2(^1S)4d\ ^2D$	2.5		30261					
39	$4s^24p^2(^3P)4d\ ^2D_a$	1.5		30970					
40	$4s^24p^2(^3P)4d\ ^2D$	2.5		31323					
41	$4s4p^4(^1S)\ ^2S_a$	0.5		32459					

Table 5. The level energies E (in 100 cm^{-1}) of the W^{40+} ion and their relative deviations Δ (in %) from the NIST [28] data.

N	CSF	J	NIST	QR		RELAC [6]		MCDF [8]	
			E	E	Δ	E	Δ	E	Δ
1	$4s^24p^4\ ^3P$	2	0	0		0		0	
2	$4s^24p^4\ ^1S$	0	721	740	2.58	875	21.40	733	1.60
3	$4s^24p^4\ ^3P$	1	7415	7436	0.28	7412	−0.05	7407	−0.10
4	$4s^24p^4\ ^1D$	2	7774	7770	−0.05	7794	0.26	7780	0.08
5	$4s^24p^3(^2P)4d\ ^3D$	2		12649		12469			
6	$4s^24p^3(^2P)4d\ ^3P$	1		12856					
7	$4s^24p^3(^2P)4d\ ^3P$	0		12893					
8	$4s^24p^3(^2P)4d\ ^3F$	3		12964		12787			
9	$4s4p^5\ ^3P$	2	14061	14177	0.82	14175	0.81		
10	$4s^24p^3(^2P)4d\ ^3F$	4		14314		14199			
11	$4s^24p4\ ^3P$	0	[15470]	15459	−0.07			15482	0.08
12	$4s^24p^3(^2P)4d\ ^3D$	3	15181	15461	1.85	15391	1.39		
13	$4s^24p^3(^2P)4d\ ^1P$	1		15619		15604			
14	$4s4p^5\ ^3P_a$	2	15952	15965	0.08	16136	1.16		
15	$4s4p^5\ ^1P$	1	16800	16819	0.11	17043	1.45		
16	$4s^24p^3(^4S)4d\ ^5D$	1		19690					
17	$4s^24p^3(^4S)4d\ ^5D$	0		19699					
18	$4s^24p^3(^2D)4d\ ^3F$	2	20515	19710	−3.92				
19	$4s^24p^3(^2D)4d\ ^3F$	3	21007	20007	−4.76	19847	−5.52		
20	$4s^24p^3(^2D)4d\ ^3G$	4		20374		20218			
21	$4s^24p^3(^2P)4d\ ^3F$	2	21296	20804	−2.31	20683	−2.88		
22	$4s^24p^3(^2D)4d\ ^3D$	3	21296	21184	−0.52	21115	−0.85		
23	$4s^24p^3(^4S)4d\ ^5D$	4		21266					
24	$4s^24p^3(^2D)4d\ ^1S$	0		21488					
25	$4s^24p^3(^2D)4d\ ^1P$	1		21498		21515			
26	$4s^24p^3(^2D)4d\ ^3P$	2		21525		21617			
27	$4s^24p^3(^4S)4d\ ^3D$	3		21566		21601			
28	$4s^24p^3(^2D)4d\ ^3P$	1		21587		21691			
29	$4s^24p^3(^2D)4d\ ^3F$	4		21730					
30	$4s^24p^3(^2D)4d\ ^3G$	5		21878		21792			
31	$4s^24p^3(^2P)4d\ ^3D$	1		22233		22344			
32	$4s^24p^3(^2P)4d\ ^3P$	2		22510		22502			
33	$4s^24p^3(^2P)4d\ ^3F_a$	3		22781					
34	$4s^24p^3(^4S)4d\ ^3D$	2		23112		23125			
35	$4s^24p^3(^4S)4d\ ^3D$	1		23239		23329			
36	$4s^24p^3(^2D)4d\ ^1F$	3		23499					
37	$4s^24p^3(^2D)4d\ ^1D$	2		23719		23845			
38	$4s4p^5\ ^3P$	0		23730					
39	$4s4p^5\ ^3P$	1		24551					
40	$4s^24p^3(^2P)4d\ ^3P_a$	0		28557					
41	$4s^24p^3(^2P)4d\ ^3P_a$	1		28750					
42	$4s^24p^3(^2P)4d\ ^1F$	3		29017					
43	$4s^24p^3(^2P)4d\ ^3D_a$	2		29043					
44	$4s^24p^3(^2P)4d\ ^3F_a$	4		29373					
45	$4s^24p^3(^2P)4d\ ^1D$	2		29558					
46	$4s^24p^3(^2P)4d\ ^3D_a$	3		30003					
47	$4s^24p^3(^2P)4d\ ^1P_a$	1		31708					

the same approach in constructing the RO basis. That RO basis was slightly different in [5].

In Table 6 the QR results are compared with the experimental level energies from the NIST database, the data from RELAC [6] and MCDHF [29] calculations and the fully relativistic results MCDF [31]. In Table 6 we present those level energy values from [31] which the authors consider as their most accurate calculation data. The MCDHF [29] results are determined using the largest CI expansion in their study, consequently, their deviations from the experimental data are the smallest ones compared to those of other results presented in [29]. One can find the detailed comparison of the QR results with other theoretical data in [5].

As one can see from Table 6, the relative deviations from the experimental values are smaller than 1% for the QR and the MCDHF [29] calculation results. The deviations of the RELAC [6] and MCDF [31] results are noticeably larger. The energy of the ground configuration $4s^24p^5\ ^2P_{1/2}$ level presented in [8] is equal to 747290 cm^{-1} and deviates from the experimental data by 0.69%. So this calculated level energy is just slightly better compared to our QR results.

The group of three levels with the same experimental energy is identified as the QR levels 20, 21 and 22, same as in [29]. The ordering of the energy levels determined in the QR approach coincides

Table 6. The level energies E (in 100 cm^{-1}) of the W^{39+} ion and their relative deviations Δ (in %) from the NIST [28] data.

N	CSF	J	NIST	QR		RELAC[6]		MCDHF[29]		MCDF[31]	
			E	E	Δ	E	Δ	E	Δ	E	Δ
1	$4s^24p^5\ ^2P$	1.5	0	0		0		0		0	
2	$4s^24p^5\ ^2P$	0.5	7422	7481	0.80	7485	0.86	7474	0.70	7461	0.53
3	$4s^24p^4(^3P)4d\ ^4D$	1.5		12222		12178		12165		12357	
4	$4s^24p^4(^3P)4d\ ^4P$	0.5		12390		12377		12347		12545	
5	$4s^24p^4(^3P)4d\ ^4D$	2.5	12322	12402	0.65	12362	0.32	12353	0.25	12540	1.77
6	$4s^24p^4(^3P)4d\ ^4F$	3.5	12520	12626	0.84	12577	0.45	12572	0.42	12745	1.80
7	$4s^24p^4(^1S)4d\ ^2D$	1.5		13278		13266		13221		13337	
8	$4s^24p^4(^3P)4d\ ^4D$	0.5		13765		13886		13810		13992	
9	$4s^24p^4(^3P)4d\ ^2P$	3.5	13754	13771	0.12	13816	0.45	13855	0.73	14066	2.27
10	$4s^24p^4(^3P)4d\ ^4F$	4.5	13811	13872	0.44	13893	0.60	13916	0.76	14063	1.83
11	$4s^24p^4(^1S)4d\ ^2D$	2.5		14910		15006		14948		15083	
12	$4s^24p^4(^3P)4d\ ^4P$	1.5	15231	15287	0.37	15406	1.15	15287	0.37	15468	1.56
13	$4s^24p^4(^3P)4d\ ^2D$	2.5	15465	15539	0.48	15655	1.23	15524	0.38	15723	1.67
14	$4s4p^6\ ^2S$	0.5	16380	16240	–0.85	16560	1.10	16470	0.55	16867	2.97
15	$4s^24p^4(^3P)4d\ ^4D$	0.5		19156				19203		19395	
16	$4s^24p^4(^3P)4d\ ^4D_a$	1.5		19541				19598		19790	
17	$4s^24p^4(^3P)4d\ ^4F$	2.5		19891		19996		19952		20126	
18	$4s^24p^4(^1D)4d\ ^2G$	3.5		19982				20040		20203	
19	$4s^24p^4(^3P)4d\ ^4D_a$	3.5		20896				21049		21221	
20	$4s^24p^4(^1D)4d\ ^2P$	1.5	21355	21162	–0.90	21406	0.24	21309	–0.22	21510	0.73
21	$4s^24p^4(^1D)4d\ ^2S$	0.5	21355	21264	–0.42	21707	1.65	21418	0.30	21759	1.89
22	$4s^24p^4(^3P)4d\ ^2D_a$	2.5	21355	21319	–0.17	21651	1.38	21433	0.37	21678	1.51
23	$4s^24p^4(^3P)4d\ ^2P$	1.5		21342		21654		21467		21683	
24	$4s^24p^4(^3P)4d\ ^2F$	2.5		21376		21599		21540		21745	
25	$4s^24p^4(^1D)4d\ ^2G$	4.5		21407		21587		21570		21726	
26	$4s^24p^4(^1D)4d\ ^2D$	2.5		21648		21897		21803		22026	
27	$4s^24p^4(^1D)4d\ ^2F$	3.5		21968		22221		22136		22349	
28	$4s^24p^4(^3P)4d\ ^2D$	1.5		23126		23462		23240		23475	
29	$4s^24p^4(^3P)4d\ ^2P_a$	0.5		23578		24025		23701		23947	
30	$4s^24p^4(^1S)4d\ ^2D_a$	1.5		28455				28682		28844	
31	$4s^24p^4(^1S)4d\ ^2D_a$	2.5		29080				29365		29515	

with the experimental energy levels order and with that of the MCDHF calculation from [29]. Nonetheless, we have to admit that the level ordering for these three levels in the RELAC and MCDF results is the same but differs from other available data.

3.6. W^{38+} *energy levels*

The krypton-like tungsten W^{38+} ion has rather simple energy spectra compared to other investigated tungsten ions. The ground configuration $4s^24p^6$ consists only of the closed shells. Furthermore, only one excited configuration $4s^24p^54d$ corresponds to our investigated configurations criteria. These two configurations produce 13 levels, and ten of them are known experimentally [28].

The calculated QR results are presented in Table 7 together with the NIST data and the RELAC [6] calculation. One can see from Table 7 that the QR level energies differ from the experimental values no more than 1%. The QR data are in better agreement with the experimental energy values compared to the RELAC [6] results, although this accuracy improvement is not so apparent when compared to the tungsten ions described in the previous sections.

3.7. Radiative transitions and electron collisions

After the level energies and their eigenfunctions are determined, they are utilized to calculate parameters of the radiative transitions, i. e. the transition line strengths *S*, oscillator strengths *gf*, transition probabilities *A* (A-values).

The emission spectra of the tungsten ions with an open 4p shell contain only few strong single lines that correspond to the electric dipole transitions from several levels [32]. Other excited levels are metastable, therefore the parameters of the higher-multipole order transitions have to be calculated. It was explained in [15, 33] that the transitions from these metastable levels to the levels of different parity, i. e. the magnetic quadrupole and electric octupole transitions must be determined along with the magnetic dipole and electric quadrupole transitions among the levels with the same parity. The parameters for these transition types are determined and included in our calculation of the radiative lifetime of the excited levels. Furthermore, the plane-waves Born approximation is used to calculate the electron-impact cross-sections and collision strengths for all investigated levels of the tungsten ions. The calculation method is described in [34]. In the current work we present only the energy levels and compare them with the experimental, semiempirical and theoretical data from other authors. Nevertheless, all calculated data, including radiative transitions and collisional excitation, can be found in the ADAMANT database (http://www.adamant.tfai.vu.lt/database).

4. Summary and conclusions

The tungsten ions with the ground configuration $4s^24p^N$ were investigated by employing the quasirelativistic Hartree–Fock approach. The extensive configuration interaction wavefunctions were used to include the correlation corrections. The complete energy spectra of the ground configuration $4s^24p^N$ and the excited configurations $4s4p^{N+1}$ and $4s^24pN^{N-1}4d$ were determined.

Table 7. The level energies *E* (in 100 cm^{-1}) of the W^{38+} ion and their relative deviations Δ (in %) from the NIST [28] data.

N	CSF	*J*	NIST	QR		RELAC[6]	
			E	*E*	Δ	*E*	Δ
1	$4s^24p^6\ ^1S$	0	0	0		0	
2	$4s^24p^54d\ ^3P$	0	12080	12077	–0.03	11987	–0.77
3	$4s^24p^54d\ ^3P$	1	12400	12488	0.71	12363	–0.30
4	$4s^24p^54d\ ^3F$	3	12640	12757	0.92	12613	–0.21
5	$4s^24p^54d\ ^3D$	2	12728	12842	0.90	12727	–0.01
6	$4s^24p^54d\ ^3F$	4	13891	13891	0.00	13866	–0.18
7	$4s^24p^54d\ ^1D$	2	14090	14072	–0.12	14071	–0.14
8	$4s^24p^54d\ ^3D$	3	14517	14524	0.05	14524	0.05
9	$4s^24p^54d\ ^3D$	1	15654	15730	0.49	15791	0.88
10	$4s^24p^54d\ ^3F$	2		19829		19859	
11	$4s^24p^54d\ ^3P$	2		21301			
12	$4s^24p^54d\ ^1P$	1	21427	21380	–0.22	21672	1.15
13	$4s^24p^54d\ ^3F_a$	3		21516		21680	

The complete energy level spectra of the investigated configurations for the ions W^{42+}, W^{41+}, W^{40+} and W^{38+}, to our best knowledge, were calculated for the first time. Our calculated level energies were compared with the experimental and available theoretical data.

For the ion W^{43+} the agreement of our quasirelativistic results with the available experimental data is similar or better compared to the results from [6, 9, 12]. Nevertheless, the results from [10, 11] for the larger part of their presented level energies are slightly more accurate. On the other hand, the data from [10, 11] are given for a comparatively small number of energy levels, and some levels existing in the NIST database are not determined. For the ion W^{42+}, only the results from [12] are closer to the experimental data compared to the QR data for a larger part of the presented levels. Nevertheless, data in [12] are presented just for a small part of complete energy level spectra for the investigated configurations.

For the ground configuration of the ions W^{41+} and W^{40+}, the accuracy of our results is similar to that of the MCDF [8]. It is even better than the accuracy of RELAC [6] results for the experimentally known levels. The agreement with the experimental data for the highly excited levels of the W^{40+} ion is worse than for the levels of W^{41+}. The accuracy of the RELAC results is similar to our results. We assume that larger CI wavefunction expansion is necessary for this ion.

The ion W^{39+} with the ground configuration $4s^24p^5$ was investigated by other authors, and the complete level energy spectrum of the excited configurations is available. Our QR results are very similar in accuracy as the results from [29] obtained using the MCDHF approach and more accurate compared to the relativistic results MCDF from [31].

The calculated eigenfunctions for the energy levels are further utilized in order to determine radiative transition properties and electron-impact excitation data using the same uniform and consistent approach. Therefore spectroscopic parameters of the tungsten ions together with the collisional data determined using the quasirelativistic approach can be promptly applied in the spectra modeling for the species with an open 4p shell in the high-temperature plasma.

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VOLFRAMO JONŲ $4s^24p^N$, $4s^24p^{N-1}4d$ IR $4s4p^{N+1}$ KONFIGŪRACIJŲ ENERGIJOS SPEKTRAI

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Santrauka

Taikant kvazireliatyvistinį Hartrio ir Foko artinį, ištirti volframo jonai nuo W^{38+} iki W^{43+}. Atlikti skaičiavimai įtraukiant koreliacinius efektus konfigūracijų sąveikos artėjime, naudota transformuotų radialiųjų orbitalių bazė. Suskaičiuotos pagrindinių konfigūracijų $4s^24p^N$ bei sužadintų konfigūracijų $4s^24p^{N-1}4d$ ir $4s4p^{N+1}$ lygmenų energijos. Gauti rezultatai palyginti su esamais eksperimentiniais ir teoriniais duomenimis. Jonams W^{42+}, W^{41+}, W^{40+} ir W^{38+} visi tiriamųjų konfigūracijų energijos lygmenų spektrai gauti pirmą kartą. Jonų W^{43+} ir W^{39+} energijos lygmenys nustatyti didesniu tikslumu, palyginti su kitų autorių duomenimis.