Quasirelativistic calculation of \(4s^24p^5, 4s^24p^44d\) and \(4s^4p^6\) configuration spectroscopic parameters for the \(W^{39+}\) ion

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Abstract

The \textit{ab initio} quasirelativistic Hartree–Fock method developed specifically for the calculation of spectral parameters of heavy atoms and highly charged ions is used to derive spectral data for the \(4s^24p^5, 4s^24p^44d\) and \(4s^4p^6\) configurations of the multicharged tungsten ion \(W^{39+}\). The relativistic effects are taken into account in the Breit–Pauli approximation for the quasirelativistic Hartree–Fock radial orbitals. The configuration interaction method is applied to include the electron correlation effects. Produced data are compared with existing experimental measurements and theoretical calculations.

Keywords: energy levels, transition probabilities, oscillator strengths, level lifetimes

1. Introduction

Metallic tungsten is becoming one of the popular materials in high-temperature devices, including fusion reactors [1, 2]. The tungsten material is difficult to vaporize. Nevertheless, the highly-charged ions of tungsten can emerge in fusion plasma causing the decrease of its temperature. Thus there is a need to control the concentration of these ions by monitoring their spectra. Only reliable theoretical data of the multicharged tungsten ion spectral properties enable to model such types of plasma providing means to its diagnostics, see e.g. [3]. On the other hand, the theoretical energy spectra and transition parameter calculations are helpful in identifying the emission lines of the multicharged tungsten ions which are observed in the specially designed experiments.

This situation has increased interest from both the experimental and theoretical physicists in study of the tungsten ions of various ionization stages. An extensive compilation of the experimental data and their semi-empirical investigation has been reported in [4]. A consequent review of the experimental and theoretical works is reported in [5]. Over the last few years, several experimental works (see, e.g. [6–9] and the references therein) on the tungsten ions are published. Alongside there is a considerable interest in multicharged ions from theoreticians. Some part of reported calculations are based on different variational methods utilizing the solutions of Dirac–Fock relativistic equations, see [10–13]. Another part of calculations [14, 15] is mainly based on the relativistic many-body perturbation theory with additional calculations in [15] performed using a quasirelativistic Hartree–Fock with the superposition of configurations and the relativistic multiconfiguration Hebrew University Lawrence Livermore Atomic Code (HULLAC). A quasirelativistic approximation (QR) developed at Vilnius University was successfully applied for the study of tungsten ions in [16–18]. The above works were devoted to the tungsten ions with an open 4d shell.

The quasirelativistic investigation of the tungsten ions with an open 4d shell [16–18] has demonstrated that our QR [19–21] is capable of producing reliable and highly-accurate spectroscopic parameters for the tungsten ions of such a high ionization degree. This conclusion gives us confidence to consider the higher ionization stages and to start investigation of the tungsten ions with an open 4p shell.

In the current work we present the results for the \(W^{39+}\) ion in the ground and the lowest two excited configurations. The relevance and actuality of the spectroscopic data for this ion is reflected in number of papers; for us new theoretical transition data open a way to compare those data to our calculation results and to assess the accuracy of determined spectroscopic parameters.
The experimental electron-beam-ion-trap (EBIT) measurements for the multicharged ions with an open 4p shell were reported in [22]. There authors employed theoretical data from [23] for the line identification. The fully relativistic parametric potential code RELAC [24] was adopted in [23] for the data production. Later on, some new lines of the W$^{39+}$ were presented in [25] where the HULLAC [26] code, analogous to the RELAC one, was used in calculations. The EBIT measurements in [27] made it possible to identify few more lines by applying the flexible atomic code [28]. Those experimental studies were summarized in [4], and the atomic data could be found in database [29].

Very recently, several new theoretical studies were reported. In those works data for the ion W$^{39+}$ ground and two lowest excited configuration level energies, the level radiative lifetimes $\tau$ and the electron transition parameters were presented. Their studies were using fully relativistic calculations with the configuration interaction (CI) approximation used to include electron-correlation effects as implemented in the computer code general-purpose relativistic atomic structure package (GRASP) [30]. The theoretical energy levels of the ground 4p$^3$ and 4d$^3$ configurations of the tungsten ions and the radiative transition parameters among their levels were calculated in [10]. The data for the excited configurations of the W$^{39+}$ were reported quite recently. The first calculation [31] results were substantially analyzed and strongly criticized in [32]. Based on the latter, the same authors presented more extensive calculation results for the W$^{39+}$ in [33]. The discussion about the relativistic calculation of the spectral parameters [34] was extended in [35], where several systematic calculations of the W$^{39+}$ were performed using different CI wavefunction expansions.

Our previous quasirelativistic calculations of the spectroscopic parameters for the tungsten ions with open 4d shell [16–18] pointed out to the high-accuracy of our transition probability values and their nice agreement with relativistic calculation results from [10] when the transitions among the the ground configuration levels were considered. Unfortunately, the lack of calculated data did not allow to compare data for the transitions from the levels of the excited configurations. Above mentioned W$^{39+}$ studies [33, 35] provided us with an impetus to perform a large-scale comparison of quasirelativistic and relativistic calculation data. In the next section we give a short description of employed quasirelativistic approach. In section 3 we compare our results with the data from other authors. The summary and conclusions are presented in section 4.

2. Description of quasirelativistic calculation

The quasirelativistic calculations are performed according to the description given in our previous papers [16–18] and the references therein. At the first stage, we solve the QR equations for the ground configuration 4s$^2$4p$^5$, see [19, 20]. Here we need to mention some peculiarities of our calculations. It was demonstrated in [20] that, for the averaging of QR equations over the one-electron angular momenta $j$, one has to improve their accuracy at the spherical $r$-coordinate origin ($r \rightarrow 0$) by accounting for the spin–orbit interaction. For that purpose, an additional parameter $X_{np}$ has been introduced. The calculations for the tungsten ions with open np shell demonstrated that the $X_{np}$ value significantly influences the values of the spin–orbit interaction parameter $\eta(4p)$. In order to improve the accuracy of the spin–orbit interaction, we have increased the parameter $X_{np}$ value by few tens of percent compared to that in [20].

At the second step, we solve the QR equations for the 4d and 4f radial orbitals (RO) in a frozen-core potential. In order to perform our calculations in a multiconfiguration approximation, the basis of determined RO is supplemented with the transformed radial orbitals (TRO), which have variable parameters [21]. The TRO are determined for the RO having the principal quantum number $n \leq 10$ and for all possible values of the orbital quantum number $l$, i.e. $l \leq 9$.

The relativistic corrections are included in the Breit–Pauli approach specially adopted for the quasirelativistic RO [21]. We employ the same RO basis both for the even and the odd configurations. Therefore we can avoid any inaccuracies of the calculated transition parameters occurring when the non-orthogonal RO are used.

The set of the admixed configurations for the CI expansion was generated by virtually exciting one or two electrons from the external 4f shell and the internal 3f shell of the adjusted configurations 4s$^2$4p$^5$, 4s$^2$4p$^4$4d and 4s$^4$4p$^5$. Such a set enables us to include comprehensively the correlation effects including the core-polarization effect. By applying this method and the generated RO basis for the ground (odd) configuration 4s$^2$4p$^5$, we can determine the total amount $M_o = 3172$ of the admixed configurations which can interact with the adjusted configuration. Further we apply the selection method for the admixed configurations. More details on this method are given in [36]. We need to mention that this method has been applied in all our previously described calculations. In the present calculation, we select $S_o = 188$ strongly-interacting configurations according to their weights in CI expansion, including the adjusted one. They produce total number of $C_o = 116008$ configuration state functions (CSF). The $C_o$ is further reduced to $R_o = 2824$ by applying the CSF reduction methods described in [37].

For the excited (even) configurations 4s$^2$4p$^4$4d and 4s$^4$4p$^5$, one can generate $M_e = 7286$ admixed configurations. Our selection methods help us to reduce this number to $S_e = 949$ most important configurations. Furthermore, the initial number of CSF $C_e = 6234470$ is reduced to $R_e = 426816$ in the same way as it is done for odd configurations.

After the two-step selection methods are applied, the determined sets of CSF are employed to compute the level energies of the W$^{39+}$ ion. In our calculations, the main limiting factor is the number of the same LS terms. It determines the size of the Hamiltonian matrices to be diagonalized. In our case of the W$^{39+}$ ion, the largest number, 71039, arises for the $^2F$ term of the even configurations. This number is close to our present computational limit. All our calculations are starting from the non-relativistic LS-coupling. After the level energies and their eigenfunctions are determined, these are
adopted to calculate the spectroscopic parameters of the radiative transitions. From these data, the level radiative lifetimes are derived. During the investigation of the multi-charged tungsten ions in [16, 17] we have noticed that the radiative lifetimes $\tau$ of some metastable levels can be affected not only by the M1 and E2 transitions among the levels of the excited configurations. Therefore we also have calculated such transitions for the W$^{39+}$ ion.

To perform our calculations, we have employed our own original computer codes together with the codes [38–40] which have been specifically adapted for our computing needs. The code from [38] was updated according to the methods presented in [41, 42].

### 3. Results and discussion

The calculated level energies are presented in table 1. The level indices, total angular momenta $J$, configurations and LS terms are also given in table 1. Presented percentage contributions of the LS terms are further applied to make level assignment. The term identification is rather rough and formal; it is executed according to the largest weight in the CI wavefunction expansion. Therefore, for some levels with the same total angular momentum $J$, the same LS term is attributed. In these instances, the LS term has additional index $'a'$.

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### Table 1. The level energies $E$ (in 100 cm$^{-1}$) of W$^{39+}$ and the main contributions to their wavefunctions (in %) from QR calculations.

| $N$ | Configuration | $J$ | % | NIST [29] | Exp [22] | Exp [25] | QR [22] | RELAC [33] | MCDF [35] | GK$_{CV}$ |
|-----|---------------|-----|---|-----------|---------|---------|--------|-----------|----------|--------|
| 1   | 4s$^2$4p$^3$$^3P$ | 1.5 | 98 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 2   | 4s$^2$4p$^3$$^3P$ | 0.5 | 98 | 7422 | 7420 | 7486 | 7461 | 7474 |
| 3   | 4s$^2$4p$^3$$^3P$ | 1.5 | 37 | 12199 | 12178 | 12357 | 12165 |
| 4   | 4s$^2$4p$^3$$^3P$ | 0.5 | 45 | 12370 | 12377 | 12545 | 12347 |
| 5   | 4s$^2$4p$^3$$^3P$ | 2.5 | 44 | 12322 | 12322 | 12379 | 12362 |
| 6   | 4s$^2$4p$^3$$^3P$ | 3.5 | 32 | 12520 | 12577 | 12745 | 12572 |
| 7   | 4s$^2$4p$^3$$^3P$ | 1.5 | 54 | 13255 | 13266 | 13337 | 13221 |
| 8   | 4s$^2$4p$^3$$^3P$ | 3.5 | 41 | 13754 | 13816 | 13992 | 13810 |
| 9   | 4s$^2$4p$^3$$^3P$ | 0.5 | 34 | 13758 | 13866 | 14066 | 13855 |
| 10  | 4s$^2$4p$^3$$^3P$ | 4.5 | 68 | 13811 | 13893 | 14063 | 13916 |
| 11  | 4s$^2$4p$^3$$^3P$ | 2.5 | 45 | 14889 | 15006 | 15083 | 14948 |
| 12  | 4s$^2$4p$^3$$^3P$ | 1.5 | 24 | 15231 | 15231 | 15201 | 15262 |
| 13  | 4s$^2$4p$^3$$^3P$ | 2.5 | 22 | 15465 | 15465 | 15446 | 15513 |
| 14  | 4s$^2$4p$^3$$^3P$ | 0.5 | 67 | 16380 | 16380 | 16268 | 16560 |
| 15  | 4s$^2$4p$^3$$^3P$ | 0.5 | 78 | 19739 | 19739 | 19790 | 19598 |
| 16  | 4s$^2$4p$^3$$^3P$ | 1.5 | 34 | 19458 | 19996 | 20126 | 19952 |
| 17  | 4s$^2$4p$^3$$^3P$ | 2.5 | 45 | 19809 | 20032 | 20040 | 19739 |
| 18  | 4s$^2$4p$^3$$^3P$ | 3.5 | 59 | 20814 | 21221 | 21221 | 21049 |
| 19  | 4s$^2$4p$^3$$^3P$ | 1.5 | 47 | 21080 | 21406 | 21510 | 21309 |
| 20  | 4s$^2$4p$^3$$^3P$ | 1.5 | 31 | 21355 | 21355 | 21353 | 21333 |
| 21  | 4s$^2$4p$^3$$^3P$ | 1.5 | 43 | 21355 | 21355 | 21355 | 21363 |
| 22  | 4s$^2$4p$^3$$^3P$ | 2.5 | 31 | 21355 | 21355 | 21355 | 21363 |
| 23  | 4s$^2$4p$^3$$^3P$ | 1.5 | 47 | 21080 | 21406 | 21510 | 21309 |
| 24  | 4s$^2$4p$^3$$^3P$ | 2.5 | 43 | 21294 | 21651 | 21745 | 21540 |
| 25  | 4s$^2$4p$^3$$^3P$ | 4.5 | 68 | 21326 | 21597 | 21726 | 21570 |
| 26  | 4s$^2$4p$^3$$^3P$ | 2.5 | 29 | 21761 | 21567 | 21897 | 22026 |
| 27  | 4s$^2$4p$^3$$^3P$ | 3.5 | 56 | 21887 | 22221 | 22349 | 22136 |
| 28  | 4s$^2$4p$^3$$^3P$ | 1.5 | 39 | 23041 | 23462 | 23475 | 23240 |
| 29  | 4s$^2$4p$^3$$^3P$ | 0.5 | 36 | 23498 | 24025 | 23947 | 23701 |
| 30  | 4s$^2$4p$^3$$^3P$ | 1.5 | 34 | 28316 | 28844 | 28682 |
| 31  | 4s$^2$4p$^3$$^3P$ | 2.5 | 37 | 28393 | 29515 | 29365 |

|         | MSD [29] | 73 | 164 | 276 | 75 |
|---------|----------|----|-----|-----|----|
| MSD [22] | 103 | 202 | 298 | 97 |
| MSD [35] | 82 | 206 | 259 | 73 |
complete for the configurations considered here. The level energy from [33] almost completely correspond to the GRASP3 results from [32]. The GKCV results are taken from [35]. These data are produced using the largest CI expansion and are the closest to the experimental level energies.

All the levels are presented according to the QR energy increasing order. Such an ordering completely agrees with that of GKCV results from [35] and also corresponds to the order of the experimental data. We must underline that, for the group of three levels with the same calculated energies, we assign the level numbers 21–23. The same assignment have been done in [35], whereas the level $J = 2.5$ from that group was given the level number 25 in [32]. As it is highlighted in [35], the ordering of some energy levels given in [23, 33] does not correspond to the ordering following from the most accurate results in [35]. Consequently, it does not correspond to the QR results. We mark those levels in the bold case in table 1. At the end of this table, we present the mean-square-deviations (MSD) determined by formula:

$$
\text{MSD} = \left( \frac{\sum_N (E_N^{\text{th}} - E_N^{\exp})^2 (2J_N + 1)}{\sum_N (2J_N + 1)} \right)^{1/2}.
$$

Since several works give different sets of energy levels and slightly different energy values, we determine the MSD for each set of the experimental level energies. These MSD are distinguished by different indices. As one can clearly see, the QR results are more accurate compared to those from [22] and [33]; their accuracy is almost the same as that of GKCV results from [35]. We must admit, that such an accuracy is achieved by applying significantly large CI wavefunction expansion compared to the expansion adopted in [35]. This is caused by the fact that our calculations employ the basis of the quasirelativistic RO, whereas the Dirac–Fock equation solutions are used in [35] and other mentioned theoretical studies. Moreover, the same RO basis is employed both for even-parity configurations and for those of odd parity. Therefore an additional correlation inclusion is necessary. So the CI expansion where the CSFs with the same parity and principal quantum numbers are included (GK2 in [35]) produces MSD$_{29}$ = 9400 cm$^{-1}$ whereas our QR calculation with the same expansion produces only MSD$_{29}$ = 35900 cm$^{-1}$.

Furthermore, we have performed a convergence test for our admixed configurations. When we increase a selection criterion by the factor of 1.5 (it leads to a smaller CI basis), MSD$_{29}$ changes to 7600 cm$^{-1}$. This value is very close to our best calculated value of MSD$_{29}$ = 7300 cm$^{-1}$. When we further increase the selection criterion by the factor of three, MSD$_{29}$ increases up to 14000 cm$^{-1}$. When the selection criterion is increased by the factor of ten, MSD$_{29}$ = 24000 cm$^{-1}$, when it is increased by the factor of 30, MSD$_{29}$ = 51200 cm$^{-1}$. We think such a behavior indicates that adapted selection criterion provides convergent and reliable data for the energy levels presented in table 1. When we decrease the selection criterion value, the number of admixed configurations increases very substantially. In turn, it requires very substantial increase of computer resources, both the memory and the time, although it does not guarantee a significant increase of the data accuracy. One can find a more detailed analysis of the convergence of correlation effects using the TRO basis in [43].

A very nice agreement is evident when we compare our QR percentage contributions from table 1 to analogous data from the table 2 in [35]. Almost all contributions agree within 1%, only for the levels 14, 20, 23, and 26 the deviations reach 2%. Usually the QR percentage contributions are slightly lower compared to those of GKCV from [35]. This happens because the larger CI wavefunction expansion is employed in our calculation.

In general, this kind of agreement of the QR and GKCV results is very encouraging as calculations are performed using basically different approximations. Likewise in QR results, GKCV calculations produce above-mentioned levels with the same main percentage contributions in the LS-coupling and their level assignment matches that of our QR data. When we compare the QR percentage contributions to those from [33], their agreement is nice also for most levels. The differences of 1–2% can be observed not only for the largest (main) contributions but also for the other most important components of eigenfunctions. We do not present these contributions in the present work. The large deviations up to 6% between the QR results and the data from [33] are

| $N$ | $J$ | QR | MCD[33] |
|-----|-----|----|---------|
| 2   | 0.5 | 1.30E + 2 | 1.31E + 2 |
| 3   | 1.5 | 3.97E − 1 | 3.22E − 1 |
| 4   | 0.5 | 8.79E − 2 | 7.15E − 2 |
| 5   | 2.5 | 7.85E − 1 | 6.34E − 1 |
| 6   | 3.5 | 3.70E + 6 | 4.76E + 6 |
| 7   | 1.5 | 4.71E + 0 | 2.68E + 0 |
| 8   | 3.5 | 2.66E + 4 | 2.24E + 4 |
| 9   | 0.5 | 2.00E − 1 | 1.04E − 1 |
| 10  | 4.5 | 4.37E + 4 | 3.70E + 4 |
| 11  | 2.5 | 8.40E + 2 | 3.06E − 1 |
| 12  | 1.5 | 2.56E − 3 | 2.36E − 3 |
| 13  | 2.5 | 1.86E − 3 | 1.75E − 3 |
| 14  | 0.5 | 1.62E − 3 | 1.66E − 3 |
| 15  | 0.5 | 1.19E − 1 | 1.22E − 1 |
| 16  | 1.5 | 5.63E − 1 | 5.11E − 1 |
| 17  | 2.5 | 2.36E − 2 | 2.07E − 2 |
| 18  | 3.5 | 2.72E + 2 | 2.60E + 2 |
| 19  | 3.5 | 1.45E + 2 | 1.36E + 2 |
| 20  | 1.5 | 1.83E − 1 | 1.32E − 3 |
| 21  | 0.5 | 4.19E − 4 | 3.71E − 4 |
| 22  | 2.5 | 5.42E − 4 | 5.21E − 4 |
| 23  | 1.5 | 7.29E − 4 | 1.00E − 3 |
| 24  | 2.5 | 2.23E + 1 | 1.73E − 2 |
| 25  | 4.5 | 2.58E + 2 | 2.45E + 2 |
| 26  | 2.5 | 9.42E − 3 | 1.66E − 2 |
| 27  | 3.5 | 2.18E + 2 | 2.05E + 2 |
| 28  | 1.5 | 1.33E − 3 | 1.22E − 3 |
| 29  | 0.5 | 8.16E − 4 | 7.44E − 4 |
| 30  | 1.5 | 6.55E − 4 | 6.22E − 4 |
| 31  | 2.5 | 7.53E − 1 | 4.37E − 1 |

Table 2. The radiative lifetimes (in ns) of the W$^{39}$ levels.

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observed for the levels 20–23, and for 26. Furthermore, similar large deviations of the percentage contributions for these levels appear when the data from [33] and [35] are compared. It must be underlined, that energy ordering for these levels given in [33] does not correspond to that of QR or GKCV calculations.

To determine the spectroscopic parameters in the QR approach, we have calculated the E1, M2 and E3 radiative transition data for the transitions between the levels of different-parity configurations. The M1 and E2 radiative transitions have been calculated between the levels of the same-parity configurations. Calculated radiative transition data are used to determine the lifetimes $\tau$ of the excited levels. These data are available from table 2 where the level indices correspond to those in table 1. The total angular momenta $J$ of the corresponding levels are also given.

In this table we compare the results of our quasirelativistic calculations with the data from [33]. The agreement is really nice for most levels. The values $\tau_{QR}$ which differ from the $\tau_{QR}$ values by more than 20% are marked in bold face. In most cases, it happens for the values where the radiative lifetimes are relatively large. As in the case of the energy spectra, the radiative lifetimes from [33] agree very well with those from [32] determined in the GRASP3 approximation. One can notice only one substantial difference. The levels 22 and 24 with $J = 2.5$ are swapped around in [33] compared to their positions in [32]. This change makes the agreement with the QR results significantly better. Nevertheless, substantial differences between our QR data and those from [33] still exists for the levels 11 and 24.

Even if we increase the selection criterion by three times and, consequently, decrease the CI wavefunction expansion, the radiative lifetime values does not change significantly. For most levels, the changes are no more than few percent. This is true both for the short-lived levels, which have large $A$-values, and for long-lived levels, which have small $A$-values. The only exclusion are the levels 11 and 24. The use of a smaller CI basis increases the radiative lifetime value to $1.02 \times 10^5$ ns for the level 11, whereas it is increases approximately by a factor of 5 for the level 24.

One more point has to be underlined when one discusses the radiative lifetimes. As it is already demonstrated in [33], there exists number of levels arising from the odd-parity configurations $4s^24p^3d^2$, $4s4p^5$, and $4s^24p^3d^2$ which are located below two high-lying even-parity levels 30 and 31. The radiative transitions to those odd-parity levels were not calculated in the present work. They were not presented in [33] also. We have to mention that the transition energies for those transitions are relatively small therefore corresponding transition probabilities can not be large. Nevertheless, determined radiative lifetimes $\tau_{QR}$ are probably slightly overestimated.

In table 3 we present the radiative transition parameters for all excited levels of the $W^{39+}$ ion configurations $4s^24p^5$, $4s^24p^4d$ and $4s4p^5$. We present only those radiative transitions probabilities $A$ which play an important role in determining the level radiative lifetimes $\tau$.

The initial and the final level indices from table 1 and the radiative transition type are given to describe a particular transition. We compare our determined transition probabilities $A_{QR}$ with the data from [35] calculated in the GK$_2$ and GK$_{CV}$ approximations and with the transition probabilities from [33].

It is worth mentioning that inclusion of the 3d-shell polarization, which corresponds transition from the approximation GK$_2$ to the GK$_{CV}$ in [35], makes the agreement of QR results and the latter data better for most transitions.

The transition probability values in the GK$_{CV}$ approximation agree with our QR data within few percent limits for more than half of considered lines. The main exclusions from that path are the radiative transitions from the levels 20 and 26 to the lowest level 1. In this case, the inclusion of the 3d-shell polarization significantly changes calculated transition probability values. Such a behavior is not observed for the remaining transitions. Transition probabilities from the levels 20 and 26 determined in the GK$_{CV}$ approximation are the only ones from [35] which differ by more than 20% from our QR results.

The comparison of the transition probabilities from [33] with our data gives a different picture. Their percentage deviation $k$

$$k = \left( \frac{A_{33}}{A_{QR}} - 1 \right) \times 100\%$$

are presented in the last column of table 3. One can see from that table that almost a half of transitions of various types agree within 10%. There is a group of 21 transitions where deviations reach up to 50%. For 9 transitions, the deviations are over 50%. Two E1 transition probabilities from the levels 11 and 24 to the level 1 are quite exceptional because their values differ by three orders of magnitude. Unfortunately these transition probabilities are not given in [35]. It is very difficult to find a reason of such an essential difference. As we have explained before, the main LS contributions in the CI wavefunction expansions for these levels agree nicely. Furthermore, there is quite good agreement of the transition probabilities from the levels 11 and 24 to other lower levels. There is one more point worth mentioning here. If one checks the $gf$ values for these particular transitions 11–1 and 24–1 given in [32], it is evident that they differ by more than one order of magnitude going from one approximation to another.

The earlier discussed change of the calculated radiative lifetime value for level 11 due to a reduced size of the CI expansion is caused by decrease of the E1 transition probability to the level 1. In the same way, the change of the level 24 lifetime is caused by the decrease of more by two orders of magnitude in the E1 transition probability value to the level 1, whereas the probability values for M1 transitions inside configuration change insignificantly. Therefore we conclude that it is necessary to perform an independent calculation in order to find correct answer.

The total M1 and E2 transition probability value $A_{M1} + A_{E2} = 7.65 \times 10^8$ s$^{-1}$ is given in [10]. This value agrees very well with our QR value $A_{M1} + A_{E2} = 7.67 \times 10^8$ s$^{-1}$.

In the present work we also have determined parameters for the E3 transition from the excited configuration levels to
Table 3. The $W^{99+}$ emission transition probabilities $A$ (in s$^{-1}$) determined in QR and several relativistic approximations and the percentage deviations $k$ (see equation 2).

|   | QR  | MCDF | MCDF | MCDF | k    |
|---|-----|------|------|------|------|
|   |     |      |      |      |      |
| 2 | 1 M1 | 7.33(06) | 7.29(06) |      | −1%  |
| 2 | 1 E2 | 3.40(05) | 3.28(05) |      | −4%  |
| 3 | 1 E1 | 2.52(09) | 3.10(09) |      | 23%  |
| 4 | 1 E1 | 1.12(10) | 1.38(10) |      | 23%  |
| 5 | 1 E1 | 1.27(09) | 1.51(09) |      | 24%  |
| 6 | 1 M2 | 1.51(02) | 1.41(02) |      | −7%  |
| 6 | 5 M1 | 9.06(01) | 6.89(01) |      | −24% |
| 6 | 1 E3 | 2.84(01) | 3.61(08) |      | 78%  |
| 7 | 1 E1 | 2.03(08) | 1.24(07) |      | 29%  |
| 8 | 1 M1 | 2.04(04) | 2.46(04) |      | 21%  |
| 8 | 1 M2 | 1.06(04) | 1.18(04) |      | 11%  |
| 8 | 6 M1 | 6.63(03) | 8.38(03) |      | 26%  |
| 9 | 1 E1 | 3.41(09) | 8.44(09) |      | 148% |
| 9 | 2 E1 | 1.59(09) | 1.18(09) |      | −26% |
| 10 | 6 M1 | 2.29(04) | 2.70(04) |      | 18%  |
| 11 | 1 E1 | 1.12(06) | 3.27(09) |      | 2.9·10^5%  |
| 11 | 7 M1 | 4.28(04) | 5.60(04) |      | 31%  |
| 12 | 1 E1 | 3.90(11) | 4.10(11) |      | 9%   |
| 13 | 1 E1 | 5.39(11) | 5.67(11) |      | 6%   |
| 14 | 1 E1 | 5.91(11) | 6.17(11) |      | −2%  |
| 14 | 2 E1 | 2.65(10) | 2.55(10) |      | −3%  |
| 15 | 1 E1 | 6.57(09) | 6.47(09) |      | −2%  |
| 15 | 2 E1 | 1.84(09) | 1.72(09) |      | −6%  |
| 16 | 2 E1 | 1.66(09) | 1.60(09) |      | −4%  |
| 17 | 1 E1 | 1.14(08) | 3.53(08) |      | 210% |
| 17 | 1 E1 | 4.24(10) | 4.03(10) |      | 14%  |
| 18 | 6 M1 | 2.87(06) | 3.00(06) |      | 5%   |
| 18 | 5 M1 | 4.66(05) | 4.81(05) |      | 3%   |
| 18 | 6 E2 | 1.26(05) | 1.34(05) |      | 7%   |
| 19 | 10 M1 | 2.77(06) | 2.95(06) |      | 7%   |
| 19 | 8 M1 | 1.99(06) | 2.08(06) |      | 4%   |
| 19 | 13 M1 | 1.29(06) | 1.28(06) |      | −1%  |
| 19 | 11 M1 | 4.97(05) | 7.02(05) |      | 41%  |
| 19 | 5 M1 | 1.28(05) | 1.35(05) |      | 6%   |
| 20 | 10 E2 | 9.66(04) | 1.06(05) |      | 10%  |
| 20 | 1 E1 | 3.54(11) | 3.57(11) |      | 115% |
| 21 | 1 E1 | 2.38(12) | 2.49(12) |      | 13%  |
| 22 | 1 E1 | 1.85(12) | 1.97(12) |      | 4%   |
| 23 | 1 E1 | 1.37(12) | 1.46(12) |      | −28% |
| 24 | 1 E1 | 3.79(07) | 5.78(10) |      | 1.5·10^5% |
| 24 | 8 M1 | 4.56(06) | 4.80(06) |      | 5%   |
| 24 | 11 M1 | 2.09(06) | 2.10(06) |      | 0%   |
| 25 | 10 M1 | 2.91(06) | 3.06(06) |      | 5%   |
| 25 | 8 M1 | 6.68(05) | 7.05(05) |      | 5%   |
| 25 | 10 E2 | 1.25(05) | 1.36(05) |      | 8%   |
| 25 | 8 E2 | 8.56(04) | 3.39(04) |      | −60% |
| 26 | 1 E1 | 1.06(11) | 1.13(11) |      | −43% |
| 27 | 10 M1 | 2.55(06) | 2.67(06) |      | 5%   |
| 27 | 8 M1 | 8.18(05) | 8.80(05) |      | 8%   |
| 27 | 11 M1 | 6.49(05) | 6.24(05) |      | −4%  |
| 27 | 13 M1 | 2.21(05) | 3.12(05) |      | 41%  |
| 27 | 11 E2 | 9.49(04) | 1.04(05) |      | 10%  |
| 27 | 10 E2 | 8.62(04) | 9.85(04) |      | 14%  |
| 27 | 17 M1 | 5.30(04) | 6.42(04) |      | 21%  |
| 28 | 2 E1 | 6.59(11) | 6.98(11) |      | 6%   |
| 28 | 1 E1 | 9.41(10) | 1.19(11) |      | 26%  |
the ground configuration. As it has been demonstrated in [16, 17], this type of the radiative transitions can significantly affect the calculated radiative lifetime $\tau$ values of the metastable levels for the tungsten and other ions with the open 4d shell. This feature occurs for the level 6 of the investigated W$^{39+}$ ion. When we include the E3 transition from the level 6 to the level 1, it changes the determined lifetime $\tau$ value by 10%. That indicates that such a transition can affect calculated branching ratios for the decay of this level.

There exists another level, the level 8, where the M2 transition to the ground configuration influences the calculated radiative lifetime $\tau$ value. For all other levels of the excited configurations 4s$^2$4p$^4$4d and 4s4p$^6$, the radiative lifetimes are well-determined by the E1, M1 and E2 transitions. We have no doubt that calculation of the M2 and E3 radiative transitions to the ground configurations is also important for the excited configuration levels of the ions with the open 4p$^N$ shell.

4. Summary and conclusions

The developed quasirelativistic approach facilitates multi-configuration calculations employing the broad CI wavefunction basis of the admixed configurations. For the inclusion of the correlation effects, the TRO is employed. The effectiveness of this approach has been proved in many previous calculations. We include almost 1000 configurations in the CI wavefunction expansion for the excited configurations with the reduced number of CSFs exceeding 400 000.

Admixed configurations are generated by the virtual excitation of electrons from the external 4f and from the inner 3f shells. This leads to the efficient inclusion of the correlation effects. As a result, the calculated level energies for the excited configurations 4s$^2$4p$^4$4d and 4s4p$^6$ agree very well with the experimental data.

Determined parameters of the radiative E1 transitions agree well with the most reliable relativistic calculations. That makes us to believe that the transition probability values for other considered transitions are accurate enough. Produced QR data make a complete set for three investigated configurations. Hence they can be applied both for the interpretation of new experimental results and for modeling spectra of high-temperature plasma.

We have demonstrated that the E3 radiative transitions along with the M2 transitions to the ground configuration 4s$^2$4p$^5$ must be included in order to determine the correct radiative lifetime values for the metastable levels of the excited configurations 4s$^2$4p$^4$4d and 4s4p$^6$. This conclusion bears similarity with the outcome from our investigation of the multicharged ions with the open 4d shell.

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Table 3. (Continued.)

| QR    | MCDF | MCDF | MCDF | GRASP[33] | k       |
|-------|------|------|------|-----------|---------|
|       | G\(\text{K}_{\text{L}}[35]\) | G\(\text{K}_{\text{C}}[35]\) |      |           |         |
| 29    | 2    | E1   | 1.21(12) | 1.34(12) | 10%     |
| 29    | 1    | E1   | 1.14(10)   | 1.62(09) | −86%    |
| 30    | 2    | E1   | 1.53(12)   | 1.61(12) | 5%      |
| 31    | 1    | E1   | 1.31(09)   | 2.27(09) | 73%     |

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