METASTABLE LEVEL PROPERTIES OF THE EXCITED CONFIGURATION 4p⁶4d⁸4f

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Metastable levels in rhodium-like ions with the ground configuration $4p^64d^9$ and the excited configurations $4p^64d^84f$ and $4p^54d^{10}$ are investigated. The *ab initio* calculations of the level energies, radiative multipole transition probabilities are performed in a quasirelativistic Hartree–Fock approximation employing an extensive configuration interaction based on quasirelativistic transformed radial orbitals. Systematic trends in the behavior of calculated radiative lifetimes of the metastable levels are studied for the ions from Z = 60 to Z = 92. The significance of the radiative transitions of higher multipole order (M2 and E3) for the calculated radiative lifetimes is demonstrated and discussed.

Keywords: quasirelativistic approach, many-electron ions, metastable levels, radiative lifetimes

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1. Introduction

Ourprevious investigation of the 4p⁵4d^{N+1} and 4p⁶4d^{N-1}4f configuration metastable levels [1] has revealed that the ions of the rhodium isoelectronic sequence have a large number of metastable levels with comparatively large radiative lifetimes. Therefore, there is an evident need for a more detailed study. The relevance and significance of the magnetic quadrupole (M2) and electric octupole (E3) transitions for such metastable levels have been quite comprehensively described in [1]. That investigation of the significance of the M2 and E3 transitions involved a large number of atoms of different ionization stages, therefore the calculations were performed without inclusion of correlation corrections.

Metastable levels, which do not have the electric dipole decay channels, are essential in the study of both astrophysical and laboratory plasmas [2, 3, 4] or in the analysis of experimental spectra of various ions [6, 7], including very important tungsten ions (see, e. g. [4, 5, 8]). As it was concluded in [2], the parameters of high multipole order radiative transitions and the radiative lifetimes of metastable levels were "essential building blocks in radiative-collisional models simulating spectra". Traditionally, the radiative lifetimes for the excited metastable levels of the ground configuration are de-

termined from the calculated electric quadrupole (E2) and magnetic dipole (M1) transition probabilities [3, 9, 10, 11]. These types of radiative transitions can also be important when the radiative lifetimes of the levels of excited configurations are calculated [1, 6, 5]. Very recently the multiconfiguration Dirac–Hartree–Fock approach was applied to determine the E1, M1, E2, and M2 transition parameters for the ions up to Z = 36 (see [12, 13] and the references therein).

Many of the excited opposite-parity configuration levels are metastable ones due to a limited number of the E1-decay channels when the ground configuration has just few levels. In such a situation, the E3 and M2 radiative transitions become important decay channels - although those transitions are traditionally considered as weak and insignificant for the calculated radiative lifetimes [6, 14, 15]. The relativistic many-body perturbation theory was employed to investigate the Fe⁹⁺ ion properties in [14]. There the details describing the rise and decay of metastable levels are given and discussed. Transitions originating from the W²⁸⁺ ion metastable levels were observed in the EBIT experiment [6]. It was concluded after additional relativistic many-body perturbation theory (RMBPT) calculations that some of the excited configuration 4p64d94f levels have "extremely long lifetimes". The radiative

transitions in Ni-like ions from Z = 30 to Z = 100 were studied in [15] using RMBPT which includes the Breit interaction.

In our earlier work [1] we have demonstrated that the metastable levels of the excited configurations also exist for the ions other than Ni-like [15] or Pd-like ions [6] that have all closed shells in the ground configurations. Similar metastable levels can exist in the ions with the ground configurations, which have open 4d shells, e. g. in the Rh-like ions with the ground configuration 4p⁶4d⁹. Unfortunately, to our best knowledge, there are no theoretical or experimental works investigating the metastable level properties of those ions.

The aim of the present work is to demonstrate how the correlation corrections can change calculated radiative lifetimes of the metastable levels. Another issue, which has emerged during our previous investigation, is the location of the 4p⁶4d⁸5s and other excited configurations. The location in the energy spectrum of the excited configurations is important as the additional decay channels can emerge for some levels of the configuration 4p⁶4d⁸4f.

Traditionally, the levels are considered as the metastable ones when the electric dipole (E1) transitions from these levels are forbidden by the selection rules for the total orbital quantum number J. The metastable levels have two important channels of the radiative decay. One channel is comprised of the magnetic dipole and electric quadrupole transitions to the levels of the same parity, usually to the levels of the same configuration; nevertheless, the transitions among the levels of different configurations with the same parity are also allowed. The second channel constitutes the magnetic quadrupole and electric octupole transitions to the levels of different-parity configurations. The strongest radiative transitions are those connecting the excited configuration levels to the ground configuration levels. Nevertheless, some radiative transitions connecting the levels of opposite-parity excited configurations can also be relatively strong and significant in the calculation of radiative lifetimes.

The object of the present investigation is the configuration $4p^64d^84f$ levels with high values of the total angular momentum *J* and their possible decay channels. We demonstrate how their relative positions in the energy spectra and their radiative properties change along the rhodium isoelectronic sequence.

The calculations were performed in the quasirelativistic (QR) Hartree–Fock approximation [16, 17], using several different configuration interaction (CI) expansion sets. As the first step, the energy spectra were calculated for the ions from Z = 48 to Z = 92adopting a small CI expansion, which consisted of few configurations for each parity. In this particular approximation (further we call it CI1), all electrons, both from configurations under study and the admixed ones, were described purely by solutions of the quasirelativistic equations [16, 17]. After the results of the energy spectra were analyzed, the subsequent investigation of the rhodium-like ions was limited to the ions starting from Z = 60. Further, at the second step, the correlation corrections were included using the extensive CI wavefunction expansion. In this case, the electrons of the admixed configurations were described by the solutions of the quasirelativistic equations and by the quasirelativistic transformed radial orbitals [18].

2. Calculation method

We use the quasirelativistic Hartree–Fock approximation in our *ab initio* calculation of the ion level energies and radiative transition parameters, such as the line strengths *S*, weighted oscillator strengths *gf*, radiative transition probabilities *A*. The quasirelativistic calculations are performed in the way described in our previous studies [19, 20]. At the start, the QR equations for the ground configuration $4p^64d^9$ are solved. Then the QR equations for the 4f and 5*l* (up to 5g) radial orbitals (RO) are solved in the frozen-core potential. The relativistic corrections are included in the Breit–Pauli approach specially adopted for the quasirelativistic radial orbitals [18]. We employ the same RO basis both for the even and odd configurations.

The correlation corrections are included by applying the CI method. In our basic approach, called CI1, the CI includes only the configurations under research. The even configurations 4p⁶4d⁹, 4p⁶4d⁸5s and 4p⁶4d⁷5s², and the odd ones 4p⁵4d¹⁰, 4p⁶4d⁸5p and 4p⁶4d⁸4f make the smallest CI expansion sets used in the calculations. No admixed configurations are included in this approach. The results obtained in this approach (CI1) are used for the rough evaluation of the energy spectra of the configurations under investigation and the radiative transitions of different multipole orders.

The subsequent CI expansion is formed from the set of the admixed configurations generated by virtually exciting one or two electrons from the 4*l* and 5*l* shells of the adjusted configurations. The virtually excited electrons up to 5g in the admixed configurations are described by the quasirelativistic RO. Although this RO basis is rather limited, the total amount of the admixed configurations, which can interact with the adjusted ground configuration, reaches 72 for Z = 60. For the complex of the odd configurations $4p^54d^{10}$ and $4p^64d^84f$, the number of possible admixed configurations are selected by selection methods [21, 22] applied

in all our previously described calculations. The selection criterion [18] is $1 \cdot 10^{-4}$. This means that all configurations with the mean weight larger than $1 \cdot 10^{-4}$ are included into the CI expansion. There are 40 admixed even configurations and 31 odd ones after the selection rules are applied for the ion Z = 60. The admixed configurations produce a very large amount of configuration state functions (CSF). This number is reduced by applying the CSF reduction methods described in [23].

For each ion in the isoelectronic sequence, its own quasirelativistic RO basis is determined, the list of admixed configurations is generated by the same virtual excitations, and the admixed configurations are selected using the same criterion. Therefore the CI expansion differs for each particular ion and the number of admixed configurations decreases with increasing nuclear charge Z. For Z = 92, the CI expansion is significantly smaller, and only 28 even configurations and 22 odd ones are selected. The results obtained by such a way are labelled as CI2.

In order to perform more accurate and reliable calculations in the multiconfiguration approximation, the basis of determined quasirelativistic RO is supplemented with the transformed radial orbitals (TRO) described by variable parameters [18, 19, 20]. The TRO are determined for the radial orbitals having the principal quantum number $6 \le n \le 10$ and for all possible values of the orbital quantum number *l*, i. e. $l \le 9$. The admixed configurations are generated by virtually exciting one or two electrons from the 4*l* and 5*l* shells of the adjusted configurations. The virtually excited electrons are described by the quasirelativistic RO ($n \le 5$ and $l \le 4$) and by the quasirelativistic TRO for the remaining virtually excited electrons.

Due to the larger basis of the RO, the number of admixed configurations is larger than that in the previous CI2 expansion. 83 even configurations and 73 odd ones are selected for the ion Z = 60 using the same selection criterion $1 \cdot 10^{-4}$. The number of admixed configurations in the CI expansion consistently decreases along the isoelectronic sequence, and for Z = 92, there are just 42 even and 39 odd admixed configurations. The results obtained by such technique are named as CI3. The comparison of the results, determined in the CI2 and CI3 approaches, indicates that the level radiative lifetime values are quite close along the isoelectronic sequence, the difference does not exceed 10%.

The calculations employing even the larger CI expansion have been performed for several selected ions in order to verify the applied approach and to prove the convergence of the CI. These results were determined using the same large base of RO as in the CI3 approach, but the selection criterion $1 \cdot 10^{-5}$ was applied. In Table 1 they are named as CI4. The number of admixed configurations in the CI4 approach reaches several hundreds for each parity. These calculations are very complex, whereas their results differ from the CI3 data only slightly. The differences among the lifetime values obtained employing different CI expansions are demonstrated in Table 1.

Table 1. The radiative lifetimes (in ns) of the W²⁹⁺ ion configuration 4d⁸4f metastable levels.

CI1	CI2	CI3	CI4
2.16E+07	1.67E+07	1.71E+07	1.70E+07
4.64E+04	4.73E+04	4.77E+04	4.80E+04
5.54E+15	2.52E+15	3.76E+15	4.27E+15
6.04E+06	6.54E+06	6.70E+06	6.75E+06
3.18E+04	3.13E+04	3.28E+04	3.30E+04
1.60E+04	1.67E+04	1.65E+04	1.66E+04
3.24E+04	3.37E+04	3.41E+04	3.44E+04
1.82E+07	1.97E+07	2.12E+07	2.18E+07
6.03E+05	6.27E+05	6.54E+05	6.56E+05
4.52E+05	4.94E+05	4.92E+05	5.01E+05
1.58E+04	1.60E+04	1.61E+04	1.62E+04
8.10E+03	8.31E+03	8.36E+03	8.40E+03
5.35E+04	4.72E+04	4.78E+04	4.81E+04
3.02E+04	2.53E+04	2.52E+04	2.51E+04
1.49E+06	1.64E+06	1.69E+06	1.72E+06
3.90E+05	4.49E+05	4.53E+05	4.64E+05
1.69E+04	1.67E+04	1.68E+04	1.68E+04
2.22E+04	2.26E+04	2.29E+04	2.31E+04
	CI1 2.16E+07 4.64E+04 5.54E+15 6.04E+06 3.18E+04 1.60E+04 3.24E+04 1.82E+07 6.03E+05 4.52E+05 1.58E+04 8.10E+03 5.35E+04 3.02E+04 1.49E+06 3.90E+05 1.69E+04	CI1CI22.16E+071.67E+074.64E+044.73E+045.54E+152.52E+156.04E+066.54E+063.18E+043.13E+041.60E+041.67E+043.24E+043.37E+041.82E+071.97E+076.03E+056.27E+054.52E+054.94E+051.58E+041.60E+048.10E+038.31E+035.35E+044.72E+043.02E+042.53E+041.49E+061.64E+063.90E+054.49E+051.69E+041.67E+042.22E+042.26E+04	CI1CI2CI32.16E+071.67E+071.71E+074.64E+044.73E+044.77E+045.54E+152.52E+153.76E+156.04E+066.54E+066.70E+063.18E+043.13E+043.28E+041.60E+041.67E+041.65E+043.24E+043.37E+043.41E+041.82E+071.97E+072.12E+076.03E+056.27E+056.54E+054.52E+054.94E+054.92E+051.58E+041.60E+041.61E+048.10E+038.31E+038.36E+035.35E+044.72E+044.78E+043.02E+042.53E+042.52E+041.49E+061.64E+061.69E+063.90E+054.49E+054.53E+051.69E+041.67E+041.68E+042.22E+042.26E+042.29E+04

We must underline that we use the *LS*-coupling scheme for the identification of all investigated levels of the rhodium isoelectronic sequence. Although this identification can vary along the sequence, we use a uniform identification according to that of the tungsten ion (Z = 74) levels.

This table contains the radiative lifetime values of the W²⁹⁺ ion metastable levels determined using different CI expansion sets. The levels discussed in the present work are included in Table 1. The averaged difference between the values determined in the CI1 approach and those from the CI2 approach is approximately 10%, the averaged difference between the values determined in the CI2 approach and the CI3 approach is approximately 6%. Further, the averaged difference between the results from the CI3 and CI4 approximations decreases to nearly 1%. So it is clear that larger CI expansions are unnecessary as the determined lifetimes of metastable levels change just very slightly. The exception is the level $4d^{8}({}^{3}F)4f^{4}I_{13/2}$ with a very large radiative lifetime. It is obvious that the convergence test fails for this level. Here the radiative transition probabilities are strongly affected by the cancellation effects causing the lifetime value to change significantly.

Definitely, the values obtained employing the large expansion CI4 are more accurate and reliable, but, for a systematic study of the rhodium-like ion properties, the results of the CI3 approach are accurate enough. Furthermore, although the number of the admixed configurations in CI3 is not very large, the total number of CSF, due to the open 4d shells, is very large even after the reduction procedure. Consequently, the calculation consumes a very large amount of computing resources. This must be considered as an important factor since we investigate an isoelectronic sequence which has a large number of ions.

As it is mentioned in the beginning of this section, our calculation method is discussed extensively in [18]. All two-electron interactions are included in the same way as it is done in the conventional Breit-Pauli approximation. For this purpose, the codes [24, 25, 26] are adapted for the quasirelativistic radial orbital peculiarities together with our own computer codes.

The level energies, radiative lifetimes and spectroscopic parameters of the E1, M1, E2, M2 and E3 transitions calculated using the CI3 approach are published in the database ADAMANT (http://www.adamant. tfai.vu.lt/database) for the ions from Z = 60 to Z = 92.

3. Results and discussion

The ground configuration of the rhodium-like ions is $4p^{6}4d^{9}$. It has two energy levels, ${}^{2}D_{_{3/2}}$ and ${}^{2}D_{_{5/2}}$. The excited configuration $4p^{5}4d^{10}$ is also quite a simple

one and has only two levels, ${}^{2}P_{1/2}$ and ${}^{2}P_{3/2}$. These two excited levels have a usual radiative decay channel through the electric dipole (E1) transitions, therefore they are not metastable levels. Further in this work, we do not discuss them. The excited configuration $4p^{6}4d^{8}4f$ has quite a large number of the levels with high values of the total angular momentum *J*. These levels can not decay to the ground configuration by the E1 transition. Therefore their radiative lifetimes can be large if the excited levels with the opposite parity, e. g. belonging to the configuration $4p^{6}4d^{8}5s$, are located above them. The location of the excited configurations, including the $4p^{6}4d^{8}5s$, $4p^{6}4d^{7}5s^{2}$ and $4p^{6}4d^{8}5p$, is discussed further in this section.

3.1. Configuration locations

At the start of our investigation, calculations in the CI1 approach along the isoelectronic sequence (from Z = 48 to Z = 92) are performed. The level energies of the even configurations 4p64d9, 4p64d85s, 4p64d75s and the odd ones 4p54d10, 4p64d85p, 4p64d84f are determined by this rather simple way. As it is described in the previous section, only the interactions between the configurations under research (adjusted configurations) are included. The CI1 results show how the configuration position changes with Z increasing. A fraction of these results is presented in Fig. 1. The levels of the odd configurations 4p⁵4d¹⁰, 4p⁶4d⁸4f and the even configurations 4p64d85s, 4p64d75s2 are plotted relative to the ground level $4p^{6}4d^{9}{}^{2}D_{5/2}$. When Z = 48, the levels of the 4p⁶4d⁸4f configuration have additional decay channels - not only those to the levels of the ground configuration. The decay channels to the levels of the 4p64d85s and 4p64d75s2 are open as these configurations are energetically close to the ground configuration and are lower than the 4p⁶4d⁸4f configuration levels. As one can see from Fig. 1, the energy difference between the 4p⁶4d⁷5s² configuration and other configurations increases rapidly. Consequently, this configuration does not have any significance for the lifetimes of the 4p64d84f levels already at Z = 52. The configuration $4p^{6}4d^{7}5s^{2}$ is located lower than the configuration $4p^{6}4d^{8}4f$ at $Z \le 60$.

Using a strict definition, the $4p^64d^84f$ levels with $J \ge 9/2$ are not metastable ones in the case of such location of the excited configuration; only the levels with J = 15/2 can be specified as metastable ones. The E1 transitions from the levels with J = 15/2 to the configurations $4p^64d^85s$ and $4p^64d^75s^2$ are forbidden by the selection rules for *J*. These transitions are allowed from the levels with J = 13/2, but they appear only for the ion Z = 48; moreover, they are weaker than the M1 and E2 transitions. For other ions, the levels





Fig. 1. Energy levels (in 10^6 cm⁻¹) of the even configurations $4p^64d^85s$, $4p^64d^75s^2$ and the odd-configuration complex $4p^64d^84f + 4p^54d^{10}$ relative to the lowest level $4p^64d^9 {}^2D_{5/2}$ of each ion.

with J = 13/2 are metastable ones because the levels of $4p^64d^75s^2$ are located higher.

Furthermore, the lifetimes of the levels with J = 13/2 are reduced because of the E2 and M1 transitions to the configuration $4p^64d^85p$ of the same parity as the $4p^64d^84f$ one. The position of the $4p^64d^85p$ configuration in the energy spectra is presented in Fig. 2. One can see from Fig. 2 that the $4p^64d^85p$ configuration is located in the same area as the $4p^64d^84f$ and $4p^54d^{10}$ configurations for the ions $Z \le 60$. Hence, for the reliable results, these configurations must be investigated as a single complex. Figures 1 and 2 demonstrate that the levels of the configuration $4p^64d^84f$ with high values of *J* can be called the metastable ones only for the ions with $Z \ge 60$.

Figures 1 and 2 present the results of the simple CI1 approach. This approach is accurate enough for the basic calculation and for the initial assessment of the determined results. In order to determine more accurate values of the radiative transition parameters, the approaches described in Section 2 with the larger CI expansions are applied for the ions from Z = 60 up to Z = 92. The results of the approaches CI2 and CI3 have been compared, and they indicate similar trends in the

Fig. 2. Energy levels (in 10^6 cm⁻¹) of the odd configurations $4p^64d^85p$ and the odd complex $4p^64d^84f + 4p^54d^{10}$ relative to the lowest level $4p^64d^9 2D_{5/2}$ of each ion.

properties of metastable levels. Nevertheless, we use the results of more reliable CI3 approach for the comprehensive study. The results CI4 are the most accurate data, but the CI4 calculations were performed only for few ions because of their complexity and large use of the computer resources.

3.2. The lifetimes of J = 15/2 levels

The configuration $4p^{6}4d^{8}4f$ has two levels with J = 15/2. The lower one is $4d^{8}({}^{3}F)4f {}^{4}I_{15/2}$ and the higher level is $4d^{8}({}^{1}G)4f {}^{2}K_{15/2}$. The radiative lifetimes of these levels are presented in Fig. 3 for the ions from Z = 60 to Z = 92.

The radiative lifetime of the lower level is very large throughout the entire isoelectronic sequence due to its location in the energy spectra. When Z = 60 and Z = 62, this level does not have radiative transitions of the calculated multipole orders (in our case up to E3) as there are no lower-lying levels with an appropriate *J*. With *Z* increasing, the energy of the level $4d^{8}({}^{3}F)^{4}f^{4}I_{15/2}$ increases. Moreover, it increases faster than the energy of some other levels. The transition probabilities for a decay of the level $4d^{8}({}^{3}F)4f^{4}I_{15/2}$ are presented in Fig. 4. The E2 transitions are denoted by circles, M1



Fig. 3. Radiative lifetimes (in ns) of the levels with J = 15/2.



Fig. 4. Transition probabilities (in s⁻¹) from the metastable level $4d^{8}({}^{3}F)4f^{4}I_{15/2}$. Black triangles and black circles denote transitions to the $4d^{8}({}^{3}F)4f^{4}I_{13/2}$, white circles show transitions to the $4d^{8}({}^{3}F)4f^{4}H_{11/2}$.

transitions are denoted by triangles in this and in other figures, presenting the transition probabilities.

Another level with J = 15/2, namely $4d^{8}({}^{1}\text{G})4f {}^{2}\text{K}_{15/2}$, is located quite high in the energy spectra. Here the radiative lifetime is determined by some dozen E2 and M1 transitions with slowly increasing transition probability values. The strongest one is the M1 transition to the $4d^{8}({}^{3}\text{F})4f {}^{4}\text{I}_{15/2}$ level. The transition probability value increases from $3.9 \cdot 10^{2} \text{ s}^{-1}$ (for Z = 60) to $8.4 \cdot 10^{5} \text{ s}^{-1}$ (for Z = 92). As it is seen from Table 1, for Z = 74 the lifetime is $4.8 \cdot 10^{4} \text{ s}^{-1}$. In general, the M1 transitions determine the radiative lifetimes of this level for all investigated Rh-like ions.

3.3. The lifetimes of J = 13/2 levels

The configuration $4p^{6}4d^{8}4f$ has five levels with J = 13/2. The radiative lifetimes of the lowest level

 $4d^{8}({}^{3}F)4f^{4}I_{13/2}$ are presented in Fig. 5. The lifetimes of this level increase with the *Z* increasing because the location of this level in the energy spectrum is going down, i. e. the energy of this level relative to the ground level decreases unlike in the case of the lowest level with J = 15/2, where the energy difference increases when the Z increases.



Fig. 5. Radiative lifetimes (in ns) of the level with J = 13/2.

The 4d⁸(³F)4f ⁴I_{13/2} level has three decay channels open when Z = 60 and Z = 62. When $Z \ge 64$, only one E2 transition to the 4d⁸(³F)4f ⁴I_{9/2} level is allowed. This transition determines the lifetimes of the level 4d⁸(³F)4f ⁴I_{13/2} up to Z = 80. For the higher Z, the decay channel to the 4d⁸(³F)4f ⁴I_{9/2} is also closed. For the ions with $Z \ge 82$, the 4d⁸(³F)4f ⁴I_{13/2} level does not have a radiative decay channel, because the radiative transitions of all calculated multipole orders to the levels, which are lower than the investigated one, are forbidden by the selection rules for J. The lifetime of this level calculated for the tungsten ion is $3.8 \cdot 10^{15} \text{ s}^{-1}$ (see Table 1), this is close to 49 days.

The lifetimes of other four levels with J = 13/2 are presented in Fig. 6. One can see from this figure that the radiative lifetimes consistently decrease going up along the sequence. The lifetimes of three levels are very similar in magnitude, but the lifetimes of the level 4d⁸(³F)4f ⁴I_{13/2} are always noticeably (by two orders of magnitude) larger. This particular level is located relatively low in the energy spectra. Nevertheless, it is located higher compared to the level 4d⁸(³F)4f ⁴I_{13/2}. The level 4d⁸(³F)4f ⁴I_{13/2} has seven allowed transitions to the lower levels, three of these being the M1 transitions and four being the E2 ones. Their transition probabilities are presented in Fig. 7.

As one can see from Fig. 7, the dependence of the transition probability A on a nuclear charge Z has a marked minimum for some lines. This is caused by



Fig. 6. Radiative lifetimes (in ns) of four levels with J = 13/2.



Fig. 7. Transition probabilities (in s⁻¹) from the level $4d^{8}({}^{3}F)4f {}^{4}I_{{}^{13/2}}$. Black triangles and circles denote transitions to the level $4d^{8}({}^{3}F)4f {}^{4}H_{{}^{11/2}}$, white triangles and circles show transitions to the level $4d^{8}({}^{3}F)4f {}^{4}I_{{}^{13/2}}$, grey triangles and circles denote transitions to the $4d^{8}({}^{3}F)4f {}^{4}I_{{}^{15/2}}$ level, blank and white circles show transitions to the $4d^{8}({}^{3}F)4f {}^{4}F_{{}^{9/2}}$ level.

cancellation effects. The radiative transition probability A is proportional to the square of the transition operator matrix element. When this matrix element changes its sign, its value becomes very close to 0 at a particular value of Z. Consequently, the square of the radiative transition operator matrix element has a sharp minimum at this Z, causing such a peculiar shape of A(Z). Similar shapes of A(Z) can also occur in other isoelectronic sequences [1]. One can see a very similar behaviour of the radiative transition parameters proportional to the square of the matrix element in [15].

Another three levels with J = 13/2 are located comparatively high in the energy spectra and have much more open decay channels. Furthermore, the strongest transition probabilities from these levels are from 10 to 100 times larger than those of the low-lying level $4d^{8}({}^{3}F)4f^{4}I_{{}^{13/2}}$. The M1 transitions are dominant, as in Fig. 7, and they determine the radiative lifetimes of the levels with J = 13/2.

3.4. The lifetimes of J = 11/2 levels

The configuration $4p^{6}4d^{8}4f$ has nine levels with J = 11/2. Figure 8 presents the radiative lifetimes of five levels, whereas the lifetimes of other four levels are in the region between the lowest two curves. The level $4d^{8}({}^{3}F)4f {}^{4}H_{11/2}$ has the largest lifetime. The transition probability values of the radiative transitions from this level are presented in Fig. 9. The M1 transition probabilities are significantly larger than the E2 transition probabilities. This feature is similar to properties of the levels with J = 13/2.



Fig. 8. Radiative lifetimes (in ns) of five levels with J = 11/2.



Fig. 9. Transition probabilities (in s⁻¹) from the level $4d^{8}({}^{3}F)4f {}^{4}H_{{}_{11/2}}$. Black triangles and circles denote transitions to the level $4d^{8}({}^{3}F)4f {}^{4}F_{{}_{9/2}}$, white triangles and circles show transitions to the level $4d^{8}({}^{3}F)4f {}^{4}I_{{}_{13/2}}$, grey circles denote transitions to the level $4d^{8}({}^{3}F)4f {}^{4}F_{{}_{7/2}}$, black squares show transitions to the $4d^{9} {}^{2}D_{5/2}$ level.

Unlike the levels with $J \ge 13/2$, this level (as well as other levels with J = 11/2) can decay to the ground configuration in accordance with the selection rules for J. This complementary decay channel is an electric octupole transition. The probabilities of the E3 transitions are marked by squares in Fig. 9 (and in the following plots as they appear). The E3 transition probability for the $4d^8({}^{3}F)4f {}^{4}H_{11/2}$ level has the largest value at the top of the investigated isoelectronic sequence. That means that the E3 transition is the dominant one in determining the radiative lifetime. The inclusion of the E3 transition probability into the radiative lifetime calculation decreases the lifetime by a factor of 1.8 at the top of the sequence. It is seen from Fig. 9 that the probabilities of two M1 transitions and one E3 transition determine the calculated radiative lifetime value of the 4d8(3F)4f 4H11/2 level because the probabilities of three E2 transitions are distinctly smaller. For the calculated lifetime of this level, the E3 transition is critical, especially at the top end of the investigated sequence, where its value is largest. Other levels with J = 11/2 also acquire an open decay channel via the E3 transition. Nonetheless, here the E3 transition probability is always somewhat smaller compared to several M1 transitions, although it is larger than the E2 transition probabilities. For these levels, the number of M1 transitions is large, but there is only one E3 transition, therefore it does not constitute a significant decay channel as it does in the case of the level 4d8(3F)4f4H11/2.

Here we must explain that all calculated transition probabilities with the values larger than $1 \cdot 10^{-18}$ s⁻¹ from the levels under consideration are included into determining of the radiative lifetime. It is important because only a limited number of transitions are allowed from the low-lying levels. If the level lies high in the energy spectra, the number of the M1 and E2 transitions is not so limited since a large number of the levels with appropriate *J* values are located lower. Since there are only two levels of the ground configuration, the number of the M2 and E3 transitions is always one or two depending on the *J* value of the initial level. Usually, the highlying levels have relatively small radiative lifetimes as they have much more open decay channels to the levels of the same configuration.

The number of the transitions to the ground configuration is determined only by the selection rules. This number does not depend on the level location in the energy spectra. The E3 transition probability values are similar in magnitude as the M1 probability values for a particular level. Nevertheless, the E3 transitions are rather insignificant decay channels for the high-lying levels as there is a large number of the M1 transitions allowed from these levels. Furthermore, the dominant M1 transition probabilities are larger for the high-lying levels, as in the case of the levels with J = 13/2.

3.5. The lifetimes of J = 9/2 levels

The configuration $4d^64d^84f$ has thirteen levels with J = 9/2. Figure 10 presents the radiative lifetimes only for six levels. The lifetimes of other seven levels are close to two curves, which present the lifetimes of levels $4d^8({}^{3}\text{F})4f {}^{4}\text{I}_{9/2}$ and $4d^8({}^{3}\text{F})4f {}^{4}\text{F}_{9/2}$ (white and gray triangles). The excluded levels are located higher than the presented ones, and their radiative lifetime dependencies on *Z* are very similar to those of the latter two levels, both in a magnitude and in a shape.

The radiative lifetimes of the lowest level $4d^{8}({}^{3}F)4f {}^{4}F_{9/2}$ (white circles) are not the largest ones, unlike the previous (J > 9/2) cases. These lifetimes are significantly smaller as there is an additional decay channel allowed by the selection rules. The transition probabilities for this level are presented in Fig. 11. One



Fig. 10. Radiative lifetimes (in ns) of six levels with J = 9/2.



Fig. 11. Transition probabilities (in s⁻¹) from the level $4d^8({}^{3}F)4f {}^{4}F_{9/2}$. Black triangles and circles denote transitions to the level $4d^8({}^{3}F)4f {}^{4}F_{7/2}$, white circles show transitions to the level $4d^8({}^{3}F)4f {}^{4}F_{9/2}$, black diamonds and squares denote transitions to the level $4d^9 {}^{2}D_{5/2}$, white squares show transitions to the level $4d^9 {}^{2}D_{3/2}$.

can notice from Fig. 11 that the M2 transition (black diamonds) to the ground configuration is the strongest one. On top of all that, two E3 transitions are allowed, and their transition probability values are larger than those of the E2 transitions. These three radiative transitions (M2 and E3) to the ground configuration are very significant. At the lower end of the investigated sequence, their inclusion decreases the calculated radiative lifetime almost by 2000 times. Further, the influence of these transitions rapidly decreases, and the inclusion of them into the radiative lifetime calculations decreases the lifetime value approximately 13 times at Z = 92. The reasons for a rapid decrease of the E3 transition values in Fig. 11 are explained in Section 3.3. According to the selection rules for J, one M2 transition and two E3 transitions are allowed from this and all other levels with J = 9/2. The number of the M1 and E2 transitions depends on the location of the level examined.

Next level with J = 9/2 is the level $4d^{8}({}^{3}F)4f {}^{2}G_{9/2}$. Black squares denote the radiative lifetime of this level in Fig. 10. Here the M2 transition is the strongest one. But the M2 transition probability value starts to decrease slowly from Z = 84. Several strong M1 transitions behave in a similar way. Such a drop of the transition probability values causes the radiative lifetime for this level to increase when $Z \ge 84$. The M2 and E3 transitions are the most significant ones at Z = 64 and Z = 66. The inclusion of their probabilities into the radiative lifetime calculations decreases the lifetime value by more than 450 times. At the top end of the sequence, this decrease drops to 3 times.

At the beginning of the sequence, the level $4d^8(^1D)4f \ ^2H_{_{9/2}}$ has the largest radiative lifetime value (see Fig. 10, black circles). The quite sharp change of the calculated lifetime for this level between Z = 80 and Z = 86 is caused by the rapid increase of the strongest M2 transition probability value together with that of several M1 transitions. Like other previously discussed levels with J = 9/2, there is one M2 transition, two E3 transitions and few M1 and E2 transitions. The M2 transition is the strongest one for Z > 70, the E3 transitions are not so strong, but their transition probability values are larger than those of the E2 transitions. The M2 and E3 transitions affect the lifetime of $4d^{8}({}^{1}F)4f^{2}H_{q/2}$, but no so significantly as the lifetimes of the previously discussed levels due to the amount of the M1 and E2 transitions allowed from this level.

The radiative lifetimes of other levels with J = 9/2, located higher in the energy spectra than the discussed ones, are determined mainly by numerous M1 transitions. The E2 transitions are also allowed, but they are much weaker than the M1 transitions. So here the influence of the E3 and M2 transitions is not so outstanding. Although these transitions cannot be discarded at all, when the nuclear charge Z is between 60 and 70, these transitions decrease the calculated lifetime value up to 4 times. Usually, the decrease drops very quickly. For heavy ions (Z > 80), the lifetime values change only by few percent.

4. Conclusions

The configurations $4p^{6}4d^{9}$, $4p^{5}4d^{10}$, $4p^{6}4d^{8}5s$, $4p^{6}4d^{7}5s^{2}$, $4p^{6}4d^{8}5p$ and $4p^{6}4d^{8}4f$ of the Rh-like ions are investigated using the quasirelativistic approach with a small CI1 expansion for the range from Z = 48 up to Z = 92. The calculation results demonstrate that the ions with Z < 60 do not have metastable levels in the excited configurations, except for two levels of the configuration $4p^{6}4d^{8}4f$ with the largest total angular momentum, J = 15/2.

The levels with J = 9/2 of the 4p⁶4d⁸5s and 4p⁶4d⁷5s² configurations are located relatively low in the energy spectra, and the E1 transitions from the 4p⁶4d⁸4f configuration levels with J < 15/2 are possible to the levels of these configurations. Furthermore, the decay channels through the M2 and E3 transitions to the 4p⁶4d⁸5s and 4p⁶4d⁷5s² are open.

On the other hand, the decay channel through the M1 and E2 transitions is open for the 4p⁶4d⁸5p configuration. For the ions with Z < 60, the configuration 4p⁶4d⁸5p is close in energy to the 4p⁶4d⁸4f and 4p⁵4d¹⁰. These energetically close and strongly interacting excited configurations must be investigated as a single configuration complex. The present investigation was devoted to the detailed investigation of the configuration 4p⁶4d⁸4f metastable levels. The 4p⁶4d⁸4f configuration levels with $9/2 \le J \le 15/2$ are metastable ones for the highly-charged ions with $Z \ge 60$. These ions are investigated thoroughly, using a large CI3 expansion within the basis of the quasirelativistic transformed radial orbitals.

The radiative lifetimes of the levels with J = 15/2 and J = 13/2 are determined by transitions to the levels with the same parity, i. e. the M1 and E2 transitions. It should be noted that the M1 transition probability values for all investigated ions are much larger (more than 100 times) than the ones of the E2 transition. The radiative lifetimes of the levels $4d^{8}({}^{3}F)4f {}^{4}I_{13/2}$ and $4d^{8}({}^{3}F)4f {}^{4}I_{13/2}$ are extremely large (more than 10 seconds) due to their position in the energy spectra. Although these two levels are relatively very low in the spectra, the level $4d^{8}({}^{3}F)4f {}^{4}I_{15/2}$ has three open radiative decay channels through rather weak transitions (one M1 and two E2). The level $4d^{8}({}^{3}F)4f {}^{4}I_{13/2}$ has only one decay channel through the E2 transition.

Since the total number of possible M1 and E2 transitions depends on a particular level location, for the high-lying levels with J = 13/2, as well as for other high-lying metastable levels, the M1 transitions

primarily determine the calculated level radiative lifetime as their probability values are significantly larger compared to those of the E2 transitions.

The lifetimes of the levels with J = 11/2 and J = 9/2 are also determined by the transitions to the levels of the same parity, but in this case, the M2 and E3 transitions to the ground configuration of the opposite parity are allowed. Since there are only two levels in the ground configuration, the number of M2 and E3 transitions is strictly defined. Only one E3 transition is possible from each level with J = 11/2; two E3 transitions and one M2 transition are allowed from each level with J = 9/2. The number of possible E2 and M1 transitions can vary depending on the location of the particular level is located higher, the number of allowed M1 and E2 transitions becomes larger.

The E3 transition probability value is similar in magnitude with that of the M1 transitions and is larger than the transition probabilities of E2 for the levels with J = 11/2. For the levels with J = 9/2, the M2 transition probability has the largest value for most ions. The E3 transition probability values are smaller than those of the M1 transitions, but are larger than the E2 transition probabilities for these levels.

The inclusion of M2 and E3 transitions into the radiative lifetime calculation can significantly change the determined total radiative lifetime value. If the level position is comparatively high in the energy spectra, the M2 and the E3 transitions are not so significant, although they cannot be neglected. For the Rh-like ions, the decay of the metastable levels through the M1 and the M2 transitions is more significant compared to the decay through the E3 ones. The E2 transition probability values are the smallest ones for all metastable levels, except for the level $4d^{8}({}^{3}F)4f {}^{4}I_{1_{3/2}}$, which can decay only through the E2 transition.

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SUŽADINTOS KONFIGŪRACIJOS 4p⁶4d⁸4f METASTABILIŲ LYGMENŲ SAVYBĖS

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Santrauka

Darbe tiriami metastabilūs sužadintos konfigūracijos 4p⁶4d⁸4f lygmenys jonuose, jų pagrindinė konfigūracija – 4p⁶4d⁹. Spektrinės charakteristikos suskaičiuotos kvazireliatyvistiniu Hartrio ir Foko artiniu atsižvelgiant į koreliacinius efektus, įskaitomus taikant konfigūracijų sąveiką skirtingose radialiųjų orbitalių bazėse. Parodyta, kad atsižvelgus į nedidelio pataisinių konfigūracijų, aprašytų tik kvazireliatyvistinių lygčių sprendiniais, skaičiaus sąveiką, gaunamos metastabilių lygmenų trukmės ženkliai skiriasi nuo trukmių, gautų atsižvelgiant tik į tiriamųjų konfigūracijų tarpusavio sąveiką. Papildžius bazę transformuotomis kvazireliatyvistinėmis orbitalėmis, gaunamos metastabilių lygmenų gyvavimo trukmės greitai konverguoja.

Atlikus pradinius skaičiavimus nedidelėje konfigūracijų bazėje, parodyta, kad jonų Z = 48-60 sužadintos konfigūracijos 4p⁶4d⁸4f lygmenys nėra metastabilūs, nes egzistuoja suirimo kanalai į žemiau esančias konfiguracijas 4p64d85s, 4p64d75s2 ir 4p64d85p. Jonams Z = 60-92 šios konfigūracijos yra energetiškai aukščiau nei tiriamoji 4p64d84f. Tokiems jonams buvo atlikti tyrimai didelėje konfigūracijų bazėje, gauti energijos lygmenų spektrai, elektrinių dipolinių, kvadrupolinių ir oktupolinių, magnetinių dipolinių ir kvadrupolinių šuolių spektroskopiniai parametrai. Išnagrinėjus metastabilių lygmenų suirimo kanalus, matyti, kad elektriniai dipoliniai šuoliai yra draudžiami atrankos taisyklių lygmenims su $J \ge 9/2$. Sių lygmenų gyvavimo trukmes lemia aukštesnio multipoliškumo šuoliai. Svarbiausi yra magnetiniai dipoliniai šuoliai, elektrinių kvadrupolinių tikimybės visada yra daug mažesnės. Kai kuriems lygmenims svarbiausi tampa elektriniai oktupoliniai ir magnetiniai kvadrupoliniai šuoliai, kurių įskaitymas ypač ženkliai sumažina lygmens gyvavimo trukmę.