

Dielectronic recombination rate coefficients of Ni-like barium and tungsten

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Abstract. *Ab initio* calculations of the total dielectronic recombination (DR) rate coefficient of Ni-like barium (Ba^{28+}) and tungsten (W^{46+}) in the ground state have been performed using the HULLAC atomic code package. Resonant and nonresonant stabilizing radiative transitions are included. Collisional transitions following electron capture are neglected. The present level-by-level calculations include the DR contributions of all of the levels (over 17000) in the Cu-like inner-shell excited configurations $3d^9 4ln'l'$ ($n' \leq 9$), $3p^5 3d^{10} 4ln'l'$ ($n' \leq 5$), and $3s3p^6 3d^{10} 4ln'l'$ ($n' \leq 5$). For both ions, the configuration complexes with a hole in the $3p$ inner shell contribute almost 10% to the total DR rate coefficient, while the complexes with a hole in the $3s$ inner shell contribute about 1%. The converging contributions of the $3d^9 4ln'l'$ ($n' > 9$) configurations are evaluated by applying the complex-by-complex n'^{-3} extrapolation method and are found to comprise up to about 20% of the total DR rate coefficients throughout a wide electron temperature range. The total DR rate coefficients are fitted to an easy-to-use analytic expression which reproduces the original data with an accuracy of about 2% or better in a very wide temperature range.

PACS. 34.80.Lx Electron recombination and electron attachment

1 Introduction

Highly ionized tungsten and barium have been the subject of many atomic physics research efforts lately. Tungsten is one of the main materials used for plasma facing divertor plates in fusion devices as in the ASDEX Upgrade tokamak [1] and is believed to be favorable for divertors in the next generation of nuclear fusion devices. Barium, on the other hand, is used in laser-produced plasma experiments where the X-ray emission from the hot plasma is studied [2–4]. The transparent BaF_2 targets are advantageous for this kind of experiments, since they eliminate the undesirable prepulse which does not interact with the target [2]. For ionization balance modeling and radiative plasma cooling studies, as well as for X-ray spectrum emission analysis, accurate atomic data for the highly ionized ions are necessary, especially data on dielectronic recombination (DR) which is the most important recombination process in highly ionized plasmas.

DR processes along the NiI isoelectronic sequence have been investigated in previous works for several ions of the sequence [5–9]. It has been shown [8] that the total DR rate coefficients have an irregular behavior along the NiI sequence, varying significantly from element to element due to the gradual lowering of inner-shell excited levels below the CuI ionization limit as the atomic number increases. This effect is very strong at low electron temperatures, but still has repercussions at high temperatures as

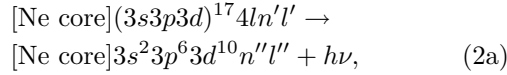
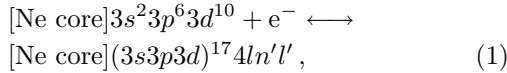
well. Hence, analysis of data along the sequence can, at the most, reveal the nonmonotonous trends due to the lowering of whole configurations below the ionization limit, but by no means can interpolation predict the abrupt irregularities from element to element due to *individual* levels. These levels when lying just above the ionization limit can dominate the whole DR rate. Therefore, when highly accurate DR data are needed, such as in tokamak plasma diagnostics, detailed level-by-level calculations still have to be performed. Also, the present results of the detailed calculations allow to evaluate the expected inaccuracies in the interpolation approximation [10]. Recently, the *partial* DR cross-sections and rate coefficients of Ni-like barium (Ba^{28+}) and tungsten (W^{46+}) through the *low-lying* inner-shell excited configurations ($3p3d$)¹⁵4l4l' were calculated [9]. In the present study, we extend these calculations for Ba and W to include all of the significant higher-lying 3l-inner-shell excited configurations as well. The calculations include the detailed contributions of all of the levels belonging to the following Cu-like inner-shell excited configuration complexes: $3d^9 4ln'l'$ ($4 \leq n' \leq 9$), $3p^5 3d^{10} 4ln'l'$ ($n' \leq 5$), and $3s3p^6 3d^{10} 4ln'l'$ ($n' \leq 5$). Aside from the detailed calculations performed for these configurations, an extrapolation method is applied to evaluate the converging contribution of the higher-lying configurations. The goal is to obtain the *total* DR rate coefficients of Ni-like Ba and W, generally following the method laid out in reference [8].

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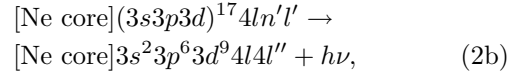
The effect of *nonresonant stabilizing* (NRS) radiative transitions from autoionizing to nonautoionizing inner-shell excited levels was systematically investigated in reference [7] for several Ni-like ions. These transitions were found to produce a significant enhancement of the effective DR through both the $3d^9 4l 4l'$ and $3d^9 4l 5l'$ complexes, especially at low electron temperatures. On the other hand, the effect of *decays* to *autoionizing* levels possibly followed by radiative *cascades* (DAC) was found to be much smaller. Consequently, in the present calculations for DR through the higher configurations, nonresonant stabilizing transitions are included, whereas decays to autoionizing levels are neglected.

2 Theoretical method

In general, the dielectronic recombination of a Ni-like ion in the ground state $3d^{10}$ can occur through any Cu-like $3l$ -inner-shell excited autoionizing level, ending at any final level below the ionization limit. This mechanism can be represented by the following main processes:



or



where $[\text{Ne core}]3s^2 3p^6 3d^{10}$ represents a Ni-like ion in the ground state, $[\text{Ne core}]$ symbolizing the full $1s^2 2s^2 2p^6$ electronic inner shells. $[\text{Ne core}](3s3p3d)^{17} 4ln'l'$ represents a Cu-like ion having a single hole in one of the $3l$ subshells. e^- is the interacting free electron and $h\nu$ an emitted photon. Process (1) is the radiationless electron capture, which is reversible by autoionization, whereas processes (2a) and (2b) are the *resonant* and *nonresonant* radiative stabilizing transitions, respectively.

The rate coefficient β_{kd} for process (1) only, *i.e.*, the capture of a free electron by a Ni-like ion in its ground state k , to form a Cu-like ion in an excited state d above the first ionization limit, can be evaluated by the principle of detailed balance. Assuming a Maxwellian electron velocity distribution corresponding to an electron temperature T_e , one obtains for the capture rate coefficient (*e.g.*, Ref. [8]):

$$\beta_{kd} = 1.656 \times 10^{-22} (kT_e)^{-3/2} \frac{g_d}{g_k} A_{dk}^a \exp\left(\frac{-E_{kd}}{kT_e}\right), \quad (3)$$

where E_{kd} is the energy difference between the level d and the first ionization limit k . E_{kd} and kT_e are expressed in eV. A_{dk}^a is the coefficient for autoionization from level d to level k , expressed in s^{-1} . g_d and g_k are the statistical

weights of the d and k levels, respectively. β_{kd} is expressed in $\text{cm}^3 \text{s}^{-1}$.

Assuming the ion does not undergo inelastic collisions with electrons after capturing the free electron, the inner-shell excited Cu-like ion in level d can either autoionize back to form a Ni-like ion or decay radiatively. This decay can be towards a level d' above the ionization limit (k) from which it can further either autoionize or decay, or it can be to a level i or d'' below the ionization limit (*i.e.* effective recombination); i denotes a $3d^{10} n'' l''$ level of the recombined Cu-like ion (process (2a)), and d'' a $3d^9 4l 4l''$ level below the ionization limit (process (2b)). Thus, considering all of these possible depletion processes from a given level d , the *branching ratio for (effective) dielectronic recombination* through the level d is defined as

$$B^D(d) = \frac{\sum_i A_{di} + \sum_{d'' < k} A_{dd''} + \sum_{d' > k} A_{dd'} B^D(d')}{\sum_{k'} A_{dk'}^a + \sum_i A_{di} + \sum_{d'' < k} A_{dd''} + \sum_{d' > k} A_{dd'}}; \quad (4)$$

$\sum A_{di}$, $\sum A_{dd''}$, and $\sum A_{dd'}$ are the sums of the Einstein coefficients for spontaneous emission from level d to levels i , d'' and d' , respectively. $\sum A_{dk'}^a$ is the total coefficient for all energetically allowed autoionizations from level d to Ni-like levels k' .

To include all the radiative decays from level d to other lower *autoionizing* levels (d') while taking into account all possible further cascades (DAC), as has been done for the $3d^9 4l 4l'$ and $3d^9 4l 5l'$ complexes [9], is computationally prohibitive for the higher complexes. In fact, these transitions in the case of the $3d^9 4l 4l'$ and $3d^9 4l 5l'$ complexes were found to have an effect of a few percent at the most; thus, by not including these processes for the higher complexes, one expects an even smaller error in the total DR rate coefficient. Disregarding the decays to autoionizing levels leads to the following approximate expression for the DR branching ratio [8]:

$$B^D(d) \approx \frac{\sum_i A_{di} + \sum_{d'' < k} A_{dd''}}{\sum_{k'} A_{dk'}^a + \sum_i A_{di} + \sum_{d'' < k} A_{dd''}}. \quad (4')$$

For the relatively low-lying d levels, the $\sum A_{dk'}^a$ sum in expressions (4) and (4') reduces to one single term A_{dk}^a : the autoionization back to the Ni-like ground state $3d^{10}$. Autoionization to excited Ni-like levels becomes substantial for the high-lying d levels, from which autoionizations to $3d^9 4l$ levels are energetically possible. All of these autoionization processes have been included in the present work.

The rate coefficient for *effective* DR, *i.e.* for process (1) plus either process (2a) or (2b), from the initial ground level k of the Ni-like ion through a given intermediate inner-shell excited level d , to any final nonautoionizing level i or d'' of the Cu-like ion is given by

$$\alpha_{kd}^D = \beta_{kd} B^D(d). \quad (5)$$

The total rate coefficient for DR from the initial level k is given by summing over all relevant d levels:

$$\alpha_k^D = \sum_d \alpha_{kd}^D. \quad (6)$$

The total number of intermediate d levels included in the present detailed level-by-level computations, pertaining to the configuration complexes $3s^23p^63d^94ln'l'$ ($4 \leq n' \leq 9$), $3s^23p^53d^{10}4ln'l'$ ($n' \leq 5$), and $3s3p^63d^{10}4ln'l'$ ($n' \leq 5$) is 17105. The $3s^23p^63d^94ln'l'$ complex series gives the most important DR contribution. Therefore, the total contribution of the higher configuration complexes with $n' > 9$ is evaluated by using a complex-by-complex extrapolation method following the n'^{-3} scaling rule, as described in reference [8]. This extrapolation method can be applied for the Ni-like ions, since the DR contributions of the whole $3d^94ln'l'$ complexes follow the n'^{-3} behavior already at relatively low- n values ($n' < 9$); this is in contrast to the slow convergence in the case of Ar-like ions for which a more sophisticated level-by-level extrapolation method is needed [11]. Configuration mixing is taken into account in the $(3s3p3d)^{17}4l4l'$ and $(3s3p)^73d^{10}4l5l'$ complexes. For higher complexes the mixing is much less important and is neglected.

The detailed level energies and radiative decay coefficients are computed using the multiconfiguration fully relativistic RELAC code [12]. The autoionization coefficients are calculated in the distorted-wave approximation using the factorization-interpolation model implemented in the HULLAC code package [13]. This method has been applied in many cases and successfully tested by comparison to more time-consuming calculation methods [13]. Unfortunately, there are no experimental DR data on the Ni-like ions studied in the present work for comparison with calculations. However, DR cross-sections of He- to C-like krypton ions computed using the HULLAC code have been compared with the DR cross-sections measured at the Berlin electron beam ion trap (EBIT), and excellent agreement with the experimental results has been obtained [14].

3 Results and discussion

In the following the results of the computations performed using detailed level-by-level calculations for Ni-like Ba^{28+} and W^{46+} are presented. Figure 1 shows the results for the total DR rate coefficients and the partial contributions of the various Cu-like inner-shell excited configuration complexes for W^{46+} as a function of the electron temperature. The general trends for Ba^{28+} are found to be similar. The detailed DR contributions of the various complexes are given in Tables 1 and 2 for both Ba^{28+} and W^{46+} , respectively, in the 10 eV to 50 keV electron temperature range. It can be seen for both ions that the $3s^23p^63d^94ln'l'$ complex series (columns 2 to 5 in the tables) gives the predominant DR contribution. The particular behavior of the rate coefficients for DR through the $3d^94l4l'$ complex along

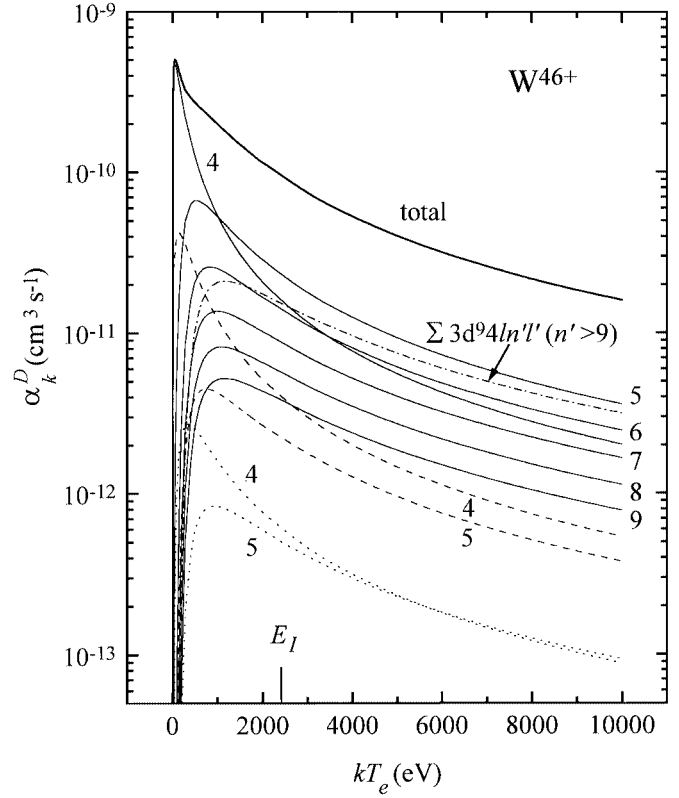


Fig. 1. Total and partial rate coefficients for DR of W^{46+} through the various Cu-like configuration complexes as a function of the electron temperature. The solid curves represent the contributions of the $3d^94ln'l'$ ($n = 4$ to 9) complexes. The dashed curves refer to the $3s^23p^53d^{10}4ln'l'$ complexes, and the dotted curves to $3s3p^63d^{10}4ln'l'$. The labels represent the values of n' in each of these cases. The dash-dotted curve represents the contribution of all the $3d^94ln'l'$ ($n' \geq 10$) complexes evaluated by extrapolation. E_1 indicates the calculated ionization energy of the Cu-like ion.

the NiI isoelectronic sequence (due to individual levels lying very close to the ionization limit) and the smoother behavior along the sequence of the DR through $3d^94l5l'$ have been discussed extensively in a previous study [7]. At low electron temperatures ($kT_e < 180$ eV for Ba and $kT_e < 450$ eV for W, *i.e.* $kT_e < 0.2E_1$ for both ions, where E_1 is the first ionization energy of the Cu-like ion) the DR process through the $3d^94l4l'$ complex is dominant (more than 50% of the total DR rate coefficient). This is due to the exponential dependence on $-E_{kd}$ (Eq. (3)) and to the small E_{kd} values in this complex. At higher electron temperatures ($kT_e > 0.4E_1$) the contribution of the $3d^94l5l'$ configuration complex becomes larger than that of $3d^94l4l'$. All of the energy levels of the $3d^94l5l'$ complex are above the ionization limit for both ions. However, they are not high enough to allow for significant autoionization to the excited $3d^94l$ Ni-like levels. Autoionization processes of this kind reduce the rate coefficients of effective DR through the high-lying complexes. Nevertheless, it can be seen from Tables 1 and 2 that the summed contributions of the $3d^94ln'l'$ complexes with $6 \leq n' \leq 9$ are

Table 1. Partial and total DR rate coefficients for Ni-like Ba as a function of the electron temperature. The rate coefficients for $3d^9 4ln'l'$ ($n' \geq 10$) were obtained by extrapolation. $X[-Y]$ denotes $X \times 10^{-Y}$.

kT_e [eV]	DR rate coefficient [$\text{cm}^3 \text{s}^{-1}$] for Ba^{28+} ($E_I = 975 \text{ eV}$)						total
	$3d^9 4l4l'$	$3d^9 4l5l'$	$3d^9 4ln'l'$ ($n' = 6$ to 9)	$3d^9 4ln'l'$ ($10 \leq n' < \infty$)	$3p^5 3d^{10} 4ln'l'$ ($n' = 4, 5$)	$3s3p^6 3d^{10} 4ln'l'$ ($n' = 4, 5$)	
10	5.78[-11]	5.57[-16]	1.43[-24]	0	9.99[-12]	2.38[-21]	6.78[-11]
20	1.34[-10]	7.74[-14]	6.47[-18]	6.00[-22]	1.18[-11]	1.31[-16]	1.45[-10]
50	1.89[-10]	4.22[-12]	1.06[-13]	2.69[-15]	1.36[-11]	9.80[-14]	2.07[-10]
100	1.69[-10]	2.33[-11]	4.19[-12]	6.00[-13]	1.84[-11]	7.96[-13]	2.15[-10]
200	1.13[-10]	5.22[-11]	2.95[-11]	9.34[-12]	2.12[-11]	1.97[-12]	2.26[-10]
500	4.52[-11]	4.80[-11]	5.53[-11]	2.60[-11]	1.48[-11]	2.00[-12]	1.90[-10]
1000	1.89[-11]	2.67[-11]	3.92[-11]	2.08[-11]	7.85[-12]	1.18[-12]	1.14[-10]
2000	7.27[-12]	1.18[-11]	1.97[-11]	1.11[-11]	3.44[-12]	5.44[-13]	5.35[-11]
5000	1.94[-12]	3.44[-12]	6.16[-12]	3.58[-12]	9.97[-13]	1.62[-13]	1.62[-11]
10000	6.97[-13]	1.27[-12]	2.34[-12]	1.37[-12]	3.69[-13]	6.05[-14]	6.07[-12]
20000	2.48[-13]	4.53[-13]	8.35[-13]	4.89[-13]	1.32[-13]	2.16[-14]	2.18[-12]
50000	6.42[-14]	1.17[-13]	2.15[-13]	1.27[-13]	3.40[-14]	5.57[-15]	5.63[-13]

Table 2. Partial and total DR rate coefficients for Ni-like W as a function of the electron temperature. The rate coefficients for $3d^9 4ln'l'$ ($n' \geq 10$) were obtained by extrapolation. $X[-Y]$ denotes $X \times 10^{-Y}$.

kT_e [eV]	DR rate coefficient [$\text{cm}^3 \text{s}^{-1}$] for W^{46+} ($E_I = 2414 \text{ eV}$)						total
	$3d^9 4l4l'$	$3d^9 4l5l'$	$3d^9 4ln'l'$ ($n' = 6$ to 9)	$3d^9 4ln'l'$ ($10 \leq n' < \infty$)	$3p^5 3d^{10} 4ln'l'$ ($n' = 4, 5$)	$3s3p^6 3d^{10} 4ln'l'$ ($n' = 4, 5$)	
10	1.79[-10]	1.36[-16]	0	0	5.61[-11]	1.17[-18]	2.35[-10]
20	3.32[-10]	1.51[-14]	3.07[-25]	0	3.06[-11]	9.21[-16]	3.62[-10]
50	4.66[-10]	5.96[-13]	6.86[-17]	4.56[-21]	2.97[-11]	1.84[-13]	4.97[-10]
100	4.31[-10]	5.94[-12]	6.18[-14]	5.09[-16]	3.98[-11]	1.03[-12]	4.78[-10]
200	3.02[-10]	2.95[-11]	3.29[-12]	2.76[-13]	4.14[-11]	2.33[-12]	3.79[-10]
500	1.26[-10]	6.64[-11]	3.68[-11]	1.04[-11]	2.85[-11]	3.14[-12]	2.73[-10]
1000	5.36[-11]	5.32[-11]	5.22[-11]	2.07[-11]	1.65[-11]	2.44[-12]	2.00[-10]
2000	2.09[-11]	2.86[-11]	3.78[-11]	1.75[-11]	7.84[-12]	1.36[-12]	1.15[-10]
5000	5.59[-12]	9.35[-12]	1.48[-11]	7.50[-12]	2.42[-12]	4.63[-13]	4.03[-11]
10000	2.02[-12]	3.60[-12]	6.05[-12]	3.16[-12]	9.15[-13]	1.81[-13]	1.60[-11]
20000	7.20[-13]	1.33[-12]	2.30[-12]	1.22[-12]	3.35[-13]	6.75[-14]	6.00[-12]
50000	1.83[-13]	3.45[-13]	6.09[-13]	3.26[-13]	8.66[-14]	1.76[-14]	1.57[-12]

still very important. The DR contribution of the very high-lying complexes $3d^9 4ln'l'$ ($n' \geq 10$) evaluated for both ions by means of the n'^{-3} complex-by-complex extrapolation method is given in the 5th column of Tables 1 and 2. In Figure 1 it is represented by the dash-dotted curve. One notices that these contributions are significant over a very wide temperature range. They represent 10% of the total DR rate coefficient already at 300 eV ($0.31E_I$) for Ba and at 950 eV ($0.39E_I$) for W, and they reach 20% at 1600 eV ($1.6E_I$) for Ba and at 9000 eV ($3.7E_I$) for W. At higher temperatures they increase very slowly.

The contributions of the DR processes through the $3s^2 3p^5 3d^{10} 4ln'l'$ ($n' = 4, 5$) complexes are shown in Figure 1 for W^{46+} by the dashed curves. The total contributions of these complexes are given in Tables 1 and 2

for both ions. These contributions are found to vary from about 8% of the total DR rate coefficient at 100 eV to about 5% at 10 keV. The contributions of the DR processes through the $3s3p^6 3d^{10} 4ln'l'$ ($n' = 4, 5$) complexes, shown in Figure 1 by the dotted curves, are found to be even smaller, *i.e.*, only about 1% of the total DR rate coefficient at temperatures above 300 eV. Since the contributions of both of the $3s^2 3p^5 3d^{10} 4ln'l'$ and $3s3p^6 3d^{10} 4ln'l'$ complex series are small, the complexes with $n' > 5$ have been disregarded here. It should be pointed out that some levels in the $3s^2 3p^5 3d^{10} 4l4l'$ complex lie close to the ionization limit and therefore their relative DR contribution is greater at very low temperatures, as can be seen, for instance, in Figure 1. In contrast, all of the $3s3p^6 3d^{10} 4ln'l'$ configurations lie high above the ionization limit, making

Table 3. Parameters obtained by a best fit of expression (7) to the total DR rate coefficients of Ni-like Ba and W calculated by detailed level-by-level computations. $X[-Y]$ denotes $X \times 10^{-Y}$.

Parameter	Ba ²⁸⁺	W ⁴⁶⁺
A_1	-25.945	-25.955
B_1	0.052198	0.027222
A_2	-24.149	-24.563
B_2	0.22292	0.11909
A_3	-22.480	-22.815
B_3	0.70063	0.55478

the autoionizations to many Ni-like $3d^9 4l$ levels possible and thus even further reducing their already small DR contribution. Finally, by summing all of the DR contributions obtained by level-by-level calculations and those evaluated by extrapolation for $3d^9 4ln'l'$ ($n' \geq 10$), the *total* DR rate coefficients are deduced. The results are presented in Tables 1 and 2 in the last column.

In prospect of an easy use for plasma modeling applications, the total DR rate coefficients are fitted to an analytic sum expression. Such an expression has already been successfully fitted to the total DR rate coefficients of other Ni-like ions [10]. The analytic expression for α_k^D , which includes six parameters, can be written as

$$\alpha_k^D = (\tau)^{-1.5} \left[\exp\left(A_1 - \frac{B_1}{\tau}\right) + \exp\left(A_2 - \frac{B_2}{\tau}\right) + \exp\left(A_3 - \frac{B_3}{\tau}\right) \right], \quad (7)$$

where τ is the reduced electron temperature kT_e/E_1 . The three exponentials reflect the average DR contributions of the low- (just above the ionization limit), intermediate-, and high-lying autoionizing Cu-like configurations. These contribute mostly at low ($\tau < 0.1$), intermediate ($\tau \cong 1$), and high ($\tau > 1$) (reduced) temperatures, respectively ($B_1 < B_2 < B_3$). The parameters obtained to best fit the DR rate coefficients of Ni-like Ba and W are given in Table 3. By using these parameters in expression (7), it is possible to reproduce the present results of the total DR rate coefficients with a very good accuracy. For temperatures $kT_e \geq 0.02E_1$, which cover the whole domain in which the ions may exist with a significant abundance in most plasmas, the discrepancies between the present level-by-level calculations and the analytical approximation (expression (7)) obtained using the parameters in Table 3 are about 2% at the most, and for most temperatures are less than 1%. It should be stressed that this accuracy is much better than the accuracy of the general formula in reference [10] where *interpolated* parameters represented by an analytic function of the ion charge are used instead of the best fit ones given here in Table 3.

4 Conclusions

Detailed level-by-level calculations of the total DR rate coefficients for ground-state Ni-like barium and tungsten have been performed and the results are presented. Non-resonant stabilizing radiative transitions are included in the calculations for all the DR channels. On the other hand, radiative decays to autoionizing levels possibly followed by cascades are included for the $3d^9 4l4l'$ and $3d^9 4l5l'$ inner-shell excited configuration complexes only. The DR contribution of the $3d^9 4ln'l'$ configuration complex series is found to be predominant. The $3d^9 4l4l'$ complex gives the main contribution at low electron temperatures due to the fact that levels of this complex lie close to the ionization limit. At high temperatures the DR contribution of the higher $3d^9 4ln'l'$ complexes becomes dominant. The DR contributions of very high complexes $3d^9 4ln'l'$ ($n' \geq 10$) is evaluated by the n'^{-3} complex-by-complex extrapolation method and is found to be significant except at low temperatures. The other two complex series $3p^5 3d^{10} 4ln'l'$ and $3s3p^6 3d^{10} 4ln'l'$ give only small DR contributions. Finally, the total DR rate coefficients computed level-by-level are fitted to a simple analytic exponential formula which reproduces the original data with an accuracy of 2% or better for $kT_e \geq 0.02E_1$.

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