Dielectronic recombination rate coefficients for highly ionized Ni-like atoms

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Ab initio calculations of the total dielectronic recombination (DR) rate coefficients for ten ions along the Ni I isoelectronic sequence in the ground state (Mo^{14+}, Ag^{19+}, Xe^{26+}, Pr^{31+}, Gd^{36+}, Dy^{38+}, Ta^{45+}, Au^{51+}, At^{57+}, and U^{64+}) have been performed using the HULLAC computer code package. Resonant and nonresonant stabilizing radiative transitions were included. Collisional transitions following electron capture were neglected. The present level-by-level calculations include the contributions of all the levels (over 17 000) belonging to the following Cu-like inner-shell excited configurations: $3d^9 4ln'l'$ ($n' \leqslant 9$), $3p^5 3d^{10} 4ln'l'$ ($n' \leqslant 5$), and $3s3p^6 3d^{10} 4ln'l'$ ($n' \leqslant 5$). The configuration complexes with a hole in the $3p$ inner shell contribute about 10% to the total DR rate coefficients and the complexes with the hole in the $3s$ inner shell about 1%. The contributions of $3d^9 4ln'l'$ for $n' > 9$ were evaluated by extrapolation, applying an n^{-3} scaling, which was checked for the specific Ta^{45+} case. It is shown that at electron temperatures higher than half the ionization energy E_I(Cu) of the Cu-like ion, the Burgess-Merts (BM) semiempirical formula can provide DR results with an accuracy better than $\pm 20\%$ for the relatively heavy ions ($Z > 54$), whereas for the lighter ions it leads to an underestimation of up to a factor 2 (for Mo). On the other hand, at low electron temperature [$kT_e < 0.3E_I$(Cu)] the BM approximation underestimates the DR rate coefficients by up to a few orders of magnitude and its temperature dependence is completely inadequate. [S1050-2947(96)07110-7]

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I. INTRODUCTION

Accurate data on recombination rates of heavy ions is essential for the study of ionization balance of highly ionized elements [1,2] and for the analysis of line intensities [3] in hot plasmas. The most important recombination process in highly ionized plasmas is the dielectronic recombination (DR). Still, precise data on DR rate coefficients for heavy ions are seldom available. Only few theoretical works have been published for DR of ions with more than 11 electrons. In the present study we investigate the DR processes throughout the Ni I isoelectronic sequence in order to obtain the total DR rate coefficients for the Ni-like ions.

In a previous work [4], *partial* rate coefficients for DR of Ni-like ions through the two particular $3d^9 4l4l'$ and $3d^9 4l5l'$ Cu-like configuration complexes were calculated. These complexes give the dominant contribution to DR at low electron temperature. In the present study we proceed with extensive *ab initio* detailed level-by-level calculations for the other significant Cu-like inner-shell excited complexes in order to obtain the *total* DR rate coefficients. The present calculations include in addition the detailed contributions of about 15 000 more levels belonging to the following Cu-like inner-shell excited configuration complexes: $3d^9 4ln'l'$ ($6 \leqslant n' \leqslant 9$), $3p^5 3d^{10} 4ln'l'$ ($n' \leqslant 5$), and $3s3p^6 3d^{10} 4ln'l'$ ($n' \leqslant 5$). All calculations are performed assuming no electron collisions occur after the initial electron capture. The present results are compared to previously published works on DR of Ni-like ions by Chen for Gd^{36+} [5] and Ta^{45+} [6] and to our previous work on Mo^{14+} [3] where only resonant radiative decays were taken into account.

The effect of *nonresonant stabilizing* (NRS) radiative transitions from autoionizing to nonautoionizing inner-shell excited levels was investigated in Ref. [4]. These transitions were found to produce a significant enhancement of the effective DR through both $3d^9 4l4l'$ and $3d^9 4l5l'$ complexes, especially at low electron temperature. On the other hand, the effect of radiative *decays* to *autoionizing* levels possibly followed by radiative *cascades* (DAC) was found to be much smaller, of the order of a few percent or even less. We will assume here that these conclusions hold for the higher inner-shell configurations considered here as well. Consequently, in the present calculations for DR through these higher configurations nonresonant stabilizing transitions have been included, whereas decays to autoionizing levels have been neglected.

Beside the detailed calculations performed for the most significant contributing configurations indicated above, a scaling rule has been applied to compute the converging contribution of the infinite number of much-higher-lying configurations. Such a rule has been proposed before [7], and its validity is checked here for the specific Ta^{45+} ion.

Until now, the large number of levels and computations that needed to be taken into account for obtaining the total DR rate coefficients had motivated the common use of the approximate semiempirical Burgess-Merts formula [8,9]. In fact, this formula was created and fitted for isoelectronic sequences very much different from the present one. The results of this approximation are compared here to the total DR

rate coefficients explicitly calculated in the present work for the Ni I sequence.

II. THEORETICAL METHOD

In general, the dielectronic recombination of a Ni-like ion in its 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 main processes

$$[\text{Ne core}]3s^2 3p^6 3d^{10} + e^- \leftrightarrow [\text{Ne core}](3s3p3d)^{17} 4ln'l', \tag{1}$$

$$[\text{Ne core}](3s3p3d)^{17} 4ln'l' \rightarrow [\text{Ne core}]3s^2 3p^6 3d^{10} n''l'' + h\nu, \tag{2a}$$

or

$$[\text{Ne core}](3s3p3d)^{17} 4ln'l' \rightarrow [\text{Ne core}]3s^2 3p^6 3d^9 4l4l'' + h\nu, \tag{2b}$$

where [Ne core]$3s^2 3p^6 3d^{10}$ represents a Ni-like ion in the ground state, [Ne core] symbolizing the full $1s^2 2s^2 2p^6$ electronic inner shells. [Ne core]$(3s3p3d)^{17} 4ln'l'$ represents a Cu-like ion having a single hole in one of the $3l$ sub-inner-shells. e^- is the interacting free electron and $h\nu$ the emitted photon. The first process is the electron capture, which is reversible by autoionization, whereas (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 (see, e.g., Ref. [10]),

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

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^a_{dk} is the coefficient for autoionization from level d to 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 $cm^3\,s^{-1}$.

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 $3d^9 4l4l''$ level below the ionization limit [process (2b)]. Thus, considering all these possible depletion processes from a given level d, the *branching ratio for (effective) dielectronic recombination* through the level d is defined as

$$B^D(d) = \frac{\Sigma_i A_{di} + \Sigma_{d''<k} A_{dd''} + \Sigma_{d'>k} A_{dd'} B^D(d')}{\Sigma_{k'} A^a_{dk'} + \Sigma_i A_{di} + \Sigma_{d''<k} A_{dd''} + \Sigma_{d'>k} A_{dd'}}. \tag{4}$$

ΣA_{di}, $\Sigma A_{dd''}$, and $\Sigma A_{dd'}$ are the sums of the Einstein coefficients for spontaneous emission from level d to levels i, d'', and d', respectively. $\Sigma A^a_{dk'}$ 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 $3d^9 4l4l'$ and $3d^9 4l5l'$ complexes [4], is computationally prohibitive for the higher complexes. In fact, these transitions in the case of the $3d^9 4l4l'$ and $3d^9 4l5l'$ complexes were found to have an effect of a few percent at most (see Sec. III A); thus, by not including these processes for the higher complexes one expects an error even smaller in the total DR rate coefficient. Disregarding the decays to autoionizing levels leads to the following approximate expression for the DR branching ratio:

$$B^D(d) \approx \frac{\Sigma_i A_{di} + \Sigma_{d''<k} A_{dd''}}{\Sigma_{k'} A^a_{dk'} + \Sigma_i A_{di} + \Sigma_{d''<k} A_{dd''}}. \tag{4'}$$

The $\Sigma A^a_{dk'}$ sum in expressions (4) and (4′) reduces for the relatively-low-lying d levels to one single term A^a_{dk}: 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 these autoionization processes have been included in the present work.

The rate coefficient for *effective* DR, i.e., for process (1) plus 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

$$\alpha^D_{kd} = \beta_{kd} B^D(d). \tag{5}$$

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

$$\alpha^D_k = \sum_d \alpha^D_{kd}. \tag{6}$$

The total number of intermediate d levels included in the present detailed level-by-level computations, pertaining to the configuration complexes $3s^2 3p^6 3d^9 4ln'l'$ ($4 \leqslant n' \leqslant 9$), $3s^2 3p^5 3d^{10} 4ln'l'$ ($n' \leqslant 5$), and $3s3p^6 3d^{10} 4ln'l'$ ($n' \leqslant 5$) is 17 105. In addition, for the $3s^2 3p^6 3d^9 4ln'l'$ ($n' > 9$) complexes an n'^{-3} extrapolation rule has been applied. Configuration mixing has been taken into account in the $(3s3p3d)^{17} 4l4l'$ and $(3s3p)^7 3d^{10} 4l5l'$ complexes. For higher complexes the mixing is much less important and has been neglected.

The detailed level energies and radiative decay coefficients were computed here using the multiconfiguration relativistic RELAC code [11]. The autoionization coefficients

TABLE I. Ratios of the rate coeffients for DR through the $3d^9 4l4l'$ and $3d^9 4l5l'$ complexes calculated in four different approximations to exact coefficients obtained by including all resonant and *nonresonant stabilizing* transitions (NRS) and *decays* to *autoionizing* levels possibly followed by radiative *cascades* (DAC), using the multiple branching ratio in Eq. (4), for Pr^{31+} and Au^{51+}. The four approximations include, respectively, *resonant stabilizing* decays only (RS); resonant and *nonresonant stabilizing* decays only (NRS); all resonant and *nonresonant* decays, but assuming that *decays* to *autoionizing* levels are followed by *autoionization* only (NRS+DAA); and all resonant and *nonresonant* decays, but assuming that *decays* to *autoionizing* levels are followed by *recombination* only (NRS+DAR).

		T_e (eV)			
Ion	Model	10	100	1000	10 000
		$3d^9 4l4l'$ complex			
Pr^{31+}	RS	0.68	0.92	0.95	0.95
	NRS	1.00	0.99	0.98	0.98
	NRS+DAA	1.00	0.98	0.98	0.97
	NRS+DAR	1.00	1.02	1.04	1.03
Au^{51+}	RS	0.95	0.97	0.98	0.98
	NRS	1.00	1.00	1.00	1.00
	NRS+DAA	1.00	1.00	1.00	1.00
	NRS+DAR	1.00	1.00	1.01	1.01
		$3d^9 4l5l'$ complex			
Pr^{31+}	RS	0.05	0.54	0.83	0.86
	NRS	1.00	0.95	0.94	0.96
	NRS+DAA	1.00	0.90	0.89	0.90
	NRS+DAR	1.00	1.13	1.19	1.20
Au^{51+}	RS	0.02	0.45	0.78	0.82
	NRS	1.00	1.00	0.99	1.00
	NRS+DAA	1.00	1.00	0.95	0.95
	NRS+DAR	1.00	1.00	1.06	1.07

were calculated in the semirelativistic distorted-wave approximation using the factorization-interpolation model implemented in the HULLAC code package [12]. This method has been applied in many cases and successfully tested by comparison to more time-consuming calculation methods [12,13].

III. RESULTS AND DISCUSSION

In the following the results of the computations performed using detailed level-by-level calculations for ten ions Mo^{14+}, Ag^{19+}, Xe^{26+}, Pr^{31+}, Gd^{36+}, Dy^{38+}, Ta^{45+}, Au^{51+}, At^{57+}, and U^{64+} of the Ni I isoelectronic sequence are presented.

A. Nonresonant radiative transitions

All the present computations take into account (after the initial electron capture) radiative decays via resonant transitions, or via *nonresonant stabilizing* (NRS) transitions, i.e., to *nonautoionizing* levels, within the $3d^9 4l4l'$ complex. In Ref. [4] it was shown that the NRS transitions do indeed give important contributions to the partial rate coefficients for DR through the $3d^9 4l4l'$ and $3d^9 4l5l'$ complexes and by no means can be ignored. The effect of *decays* to *autoionizing* levels possibly followed by *cascades* (DAC) was also investigated in that work and was found to be minor relative to the NRS effect. Since for all the high-lying inner-shell excited configurations considered here it is not practical to include all the DAC processes involving thousands of autoionizing levels, one has checked various approximations to evaluate their effect.

It is interesting to note that completely neglecting DAC transitions ($d \rightarrow d'$), which appear in expression (4) both in the numerator and in the denominator of the branching ratio, gives a fairly good approximation. As explained in Ref. [4], including DAC means adding the term $\Sigma A_{dd'} B^D(d')$ to the numerator and the term $\Sigma A_{dd'}$ to the denominator of the DR branching ratio expression [compare expressions (4) and (4′)]. On the average, one can assume that for a given ion the DR branching ratio for the different levels is more or less constant; thus the above simplification should have no influence, because in this approximation the term added to the numerator is smaller than the term added to the denominator by the same ratio as the original ratio $B^D(d)$.

In order to illustrate this feature and to compare the results of the various approximations, the ratios of the rate coefficients for DR through $3d^9 4l4l'$ and $3d^9 4l5l'$ obtained in four different approximations to the rate coefficients obtained by accurately including NRS and DAC processes are given in Table I for Pr^{31+} and Au^{51+}. In the first line only the *resonant stabilizing* (RS) transitions are included. The other three approximations all include resonant and NRS transitions, but differ by the methods for evaluating the decays to autoionizing levels. In the second approximation, decays to autoionizing levels are completely disregarded and only NRS transitions are included, i.e., as in expression (4′). In the third approximation all *decays* to *autoionizing* levels are in-

TABLE II. Total DR rate coefficients (in $cm^3\ s^{-1}$) for Mo^{14+}, Pr^{31+}, and Au^{+51} including NRS transitions (and the most important DAC processes) at different electron temperatures, compared to results of computations where only resonant transitions (RS) were taken into account. $X[-Y]$ denotes $X\times10^{-Y}$.

		T_e (eV)			
Ion	Model	10	100	1000	10 000
Mo^{14+}	present work	2.26[−11]	7.59[−11]	1.32[−11]	
	RS only [3]	8.95[−12]	5.25[−11]	1.08[−11]	
Pr^{31+}	present work	2.79[−10]	2.88[−10]	1.38[−10]	7.88[−12]
	RS only	1.98[−10]	2.50[−10]	1.18[−10]	6.88[−12]
Au^{51+}	present work	2.22[−9]	7.65[−10]	2.15[−10]	1.83[−11]
	RS only	2.11[−9]	7.26[−10]	1.83[−10]	1.58[−11]

cluded, but are assumed to be followed by *autoionization* only, i.e., $B^D(d')$ in expression (4) is taken to be zero. In the fourth approximation one assumes, to the contrary, that all *decays* to *autoionizing* levels are followed by radiative decay and ultimately by *recombination* only, i.e., $B^D(d')$ in expression (4) is taken to be unity.

The results in Table I clearly show that the NRS approximation gives the best DR predictions for the $3d^9 4l 4l'$ and $3d^9 4l 5l'$ configuration complexes, i.e., closest to the accurate calculations that take all the DAC processes into account. Similar calculations for the other Ni-like ions [14] show that this conclusion holds for the rest of the sequence as well. Thus, in the present calculations for DR through the higher complexes $3d^9 4l n'l'$ ($n' \geqslant 6$) and $3p^5 3d^{10} 4l 4l'$ (for which NRS radiative transitions are allowed), only resonant and NRS transitions have been included, but DAC processes were completely neglected. The present DR calculations for the $3d^9 4l 4l'$ and $3d^9 4l 5l'$ complexes, however, do still include DAC.

Table I shows that the commonly used RS approximation can lead to drastic underestimations for $3d^9 4l 5l'$ at low temperature. Calculations show that this is also the case for higher complexes. In order to show the overall effect of the nonresonant transitions (generally NRS, and for the $3d^9 4l 4l'$ and $3d^9 4l 5l'$ complexes DAC also) on the *total* DR rate coefficients, the results obtained for Mo^{14+}, Pr^{31+}, and Au^{51+} are compared in Table II to the results of our previous model [3], obtained with the same method, but taking only resonant transitions (RS) into account. It can be seen that at low electron temperature the nonresonant transitions enhance the total DR rate coefficient by a factor of up to about 2 for relatively light elements and at high temperature by the order of 20% for all ions. This effect is mainly due to the NRS transitions that open a large number of effective DR channels through Cu-like inner-shell excited configurations from which the resonant decays are electric-dipole forbidden (e.g., $3d^9 4s n'd$) [4]. When NRS transitions are neglected these configurations have no DR contribution at all.

B. Contribution of the various configuration complexes

Figures 1 and 2 show the results for the total DR rate coefficient and the partial contributions of the various Cu-like inner-shell excited configuration complexes for two ions Pr^{31+} and Au^{51+}, from two different ranges of the isoelectronic sequence, as a function of the electron temperature. The total rate coefficients also include the contributions of the higher complexes $3d^9 4l n'l'$ ($n' > 9$) evaluated by extrapolation as discussed in Sec. III C. The particular behavior of the rate coefficients for DR through the $3d^9 4l 4l'$ complex due to individual levels very close to the ionization limit for certain ions and the more typical behavior of DR through $3d^9 4l 5l'$ have been discussed extensively in a previous paper [4]. At low electron temperature ($kT_e < 500$ eV for Pr and $kT_e < 1000$ eV for Au) the DR process through the $3d^9 4l 4l'$ complex is predominant. This is due to the small E_{kd} values in this complex. At higher electron temperature the contribution of the $3d^9 4l 5l'$ configuration complex becomes larger. All the energy levels of this complex are above the ionization limit. However, they are not high enough to be significantly affected by autoionization to the excited $3d^9 4l$ Ni-like levels. This kind of autoionization processes can reduce

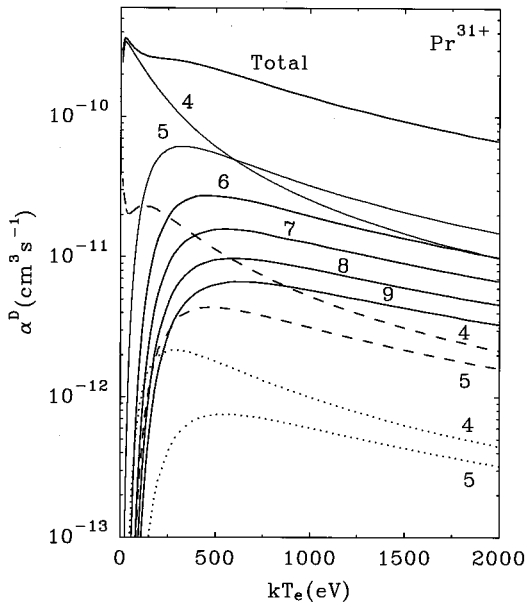

FIG. 1. Total and partial rate coefficients for DR of Pr^{31+} through the various Cu-like configuration complexes as a function of the electron temperature. The solid curves represent the contributions of the $3d^9 4l n'l'$ complexes and labels 4–9 represent values of n'. The dashed curves refer to the $3s^2 3p^5 3d^{10} 4l n'l'$ complexes and the dotted curves to $3s 3p^6 3d^{10} 4l n'l'$.

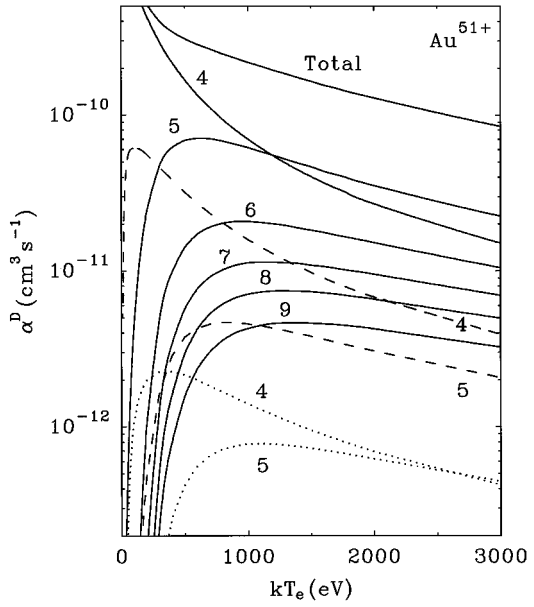

FIG. 2. Total and partial rate coefficients for DR of Au^{51+} through the various Cu-like configuration complexes as a function of the electron temperature. The solid curves represent the contributions of the $3d^9 4ln'l'$ complexes and the labels 4–9 represent the value of n'. The dashed curves refer to the $3s^2 3p^5 3d^{10} 4ln'l'$ complexes and the dotted curves to $3s3p^6 3d^{10} 4ln'l'$.

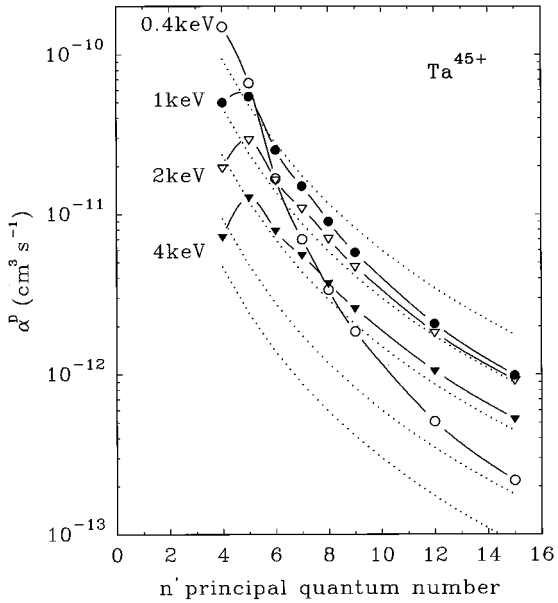

FIG. 3. Partial rate coefficients for DR of Ta^{45+} through the various $3d^9 4ln'l'$ configuration complexes as a function of the principal quantum number n' in the $n'=4$–15 range, for four selected temperatures. The solid curves are plotted through the calculated values just to guide the eye. The dotted curves indicate the n'^{-3} grid as reference for the scaling of the partial rate coefficients.

the effective DR rates through the higher-lying complexes. The DR process through the $3s^2 3p^5 3d^{10} 4ln'l'$ ($n'=4,5$) complexes is found to contribute altogether about 10% of the total DR rate and the $3s3p^6 3d^{10} 4ln'l'$ ($n'=4,5$) complexes about 1%. These contributions are shown in Figs. 1 and 2 by the dashed and dotted curves, respectively. Since these contributions are small, the $3s^2 3p^5 3d^{10} 4ln'l'$ and $3s3p^6 3d^{10} 4ln'l'$ complexes with $n'>5$ have been totally disregarded here. In some cases, levels from the $3s^2 3p^5 3d^{10} 4l4l'$ complex can lie close to the ionization limit and therefore give a significant DR effect at very low temperature, as can be seen for Pr in Fig. 1. The $3s3p^6 3d^{10} 4ln'l'$ configurations lie high above the ionization limit, making the autoionizations to many Ni-like $3d^9 4l$ levels possible. This process is especially important for the relatively low-Z elements. The distribution of the various complex contributions to the total DR rate coefficient presented here for Ni-like praseodymium and gold is found to be quite representative of the general distribution trend throughout the isoelectronic sequence.

C. Extrapolation of the $3d^9 4ln'l'$ contributions for $n'>9$

In order to estimate the DR contribution of the most significant higher complexes $3d^9 4ln'l'$ ($10 \leqslant n' < \infty$), an extrapolation approximation proposed by Hahn [7] has been used. The scaling of the partial rate coefficient $\alpha^D(n')$ for DR through a given $3d^9 4ln'l'$ complex for high-n' values can be deduced from the scalings of the coefficients for autoionization (A^a_{dk}) and radiative decays (A_{di} and $A_{dd''}$). The sums $\Sigma A^a_{dk'}$ and $\Sigma A_{dd''}$ (for $n'l' \rightarrow 4l''$ decays) appearing in expression (4′) scale as n'^{-3}. The sum ΣA_{di} (for $3d^9 4ln'l' \rightarrow 3d^{10} n''l''$) includes the coefficients of two types of radiative decays: the coefficients for $n'l' \rightarrow 3d$ decays scale as n'^{-3} (for high n') and those of $4l \rightarrow 3d$ decays are approximately independent of n' and tend to a constant. Thus, for high values of n' both the numerator and the denominator of the branching ratio for DR [expression (4′)] asymptotically tend to a constant. The n' behavior of α^D_{kd} therefore depends on β_{kd} alone. Assuming that E_{kd} is approximately constant for sufficiently high values of n', the exponent in the expression for β_{kd} [Eq. (3)] is also constant and the only dependence on n' comes from A^a_{dk}, which scales as n'^{-3}. Thus β_{kd} scales as n'^{-3} and so does α^D_{kd}. The condition for the exponent in Eq. (3) to be approximately constant is expected to be fulfilled for smaller values of n' as the electron temperature is higher, since at high temperature the exponent is less sensitive to the changes of E_{kd} as n' varies.

Denoting by n_s the lower n' value from which $\alpha^D(n')$ scales accurately enough as n'^{-3}, one can write

$$\sum_{n'=4}^{\infty} \alpha^D(n') = \sum_{n'=4}^{n_s} \alpha^D(n') + \sum_{n'=n_s+1}^{\infty} \left(\frac{n'}{n_s}\right)^{-3} \alpha^D(n_s). \tag{7}$$

The rarely addressed but important problem is to find the value of n_s. Results of recent calculations for He-like ions [15] were found to still deviate from the n'^{-3} scaling for $5 \leqslant n' \leqslant 8$; therefore it is essential to check the validity of this scaling and determine n_s for the Ni I sequence. For this purpose the Ta^{45+} ion has been taken as a sample. The contributions of the $3d^9 4ln'l'$ complexes in the $4 \leqslant n' \leqslant 15$ range have been calculated and plotted in Fig. 3. Configurations with $l'>8$ give a very small contribution and have been neglected. It can be seen that the solid curves through the calculated values tend to follow the dotted n'^{-3} grid as the

TABLE III. Total DR rate coefficients (in $cm^3\ s^{-1}$) for the ten Ni-like ions considered, as a function of the electron temperature. E_I(Cu) is the calculated ionization energy of the Cu-like ion. $X[-Y]$ denotes $X\times10^{-Y}$.

Ion	E_I(Cu) (eV)	T_e (eV) 10	20	50	100	200	500	1000	2000	5000	10 000
Mo^{14+}	301.1	2.26[−11]	3.77[−11]	6.14[−11]	7.59[−11]	6.41[−11]	3.00[−11]	1.32[−11]	5.22[−12]	1.41[−12]	5.10[−13]
Ag^{19+}	499.3	1.07[−10]	8.86[−11]	9.90[−11]	1.25[−10]	1.36[−10]	8.45[−11]	4.16[−11]	1.75[−11]	4.91[−12]	1.80[−12]
Xe^{26+}	855.7	5.66[−10]	3.28[−10]	2.26[−10]	2.08[−10]	2.17[−10]	1.73[−10]	9.95[−11]	4.56[−11]	1.35[−11]	5.07[−12]
Pr^{31+}	1168	2.79[−10]	3.55[−10]	3.34[−10]	2.88[−10]	2.62[−10]	2.19[−10]	1.38[−10]	6.71[−11]	2.08[−11]	7.88[−12]
Gd^{36+}	1531	5.08[−10]	5.59[−10]	4.51[−10]	3.61[−10]	2.93[−10]	2.39[−10]	1.62[−10]	8.41[−11]	2.71[−11]	1.05[−11]
Dy^{38+}	1690	8.02[−10]	8.25[−10]	5.45[−10]	4.11[−10]	3.27[−10]	2.60[−10]	1.79[−10]	9.43[−11]	3.09[−11]	1.20[−11]
Ta^{45+}	2315	1.87[−10]	2.70[−10]	4.19[−10]	4.31[−10]	3.57[−10]	2.70[−10]	1.99[−10]	1.14[−10]	3.98[−11]	1.57[−11]
Au^{51+}	2938	2.22[−9]	1.54[−9]	1.02[−9]	7.65[−10]	5.16[−10]	3.09[−10]	2.18[−10]	1.29[−10]	4.68[−11]	1.88[−11]
At^{57+}	3650	2.88[−9]	2.41[−9]	1.63[−9]	1.09[−9]	6.58[−10]	3.37[−10]	2.30[−10]	1.40[−10]	5.35[−11]	2.20[−11]
U^{64+}	4601	7.04[−9]	4.88[−9]	2.51[−9]	1.40[−9]	7.41[−10]	3.33[−10]	2.20[−10]	1.41[−10]	5.74[−11]	2.43[−11]

value of n' increases, confirming the validity of the scaling rule in the present case for high-n' values. For $kT_e=4$ keV the n'^{-3} scaling becomes quite appropriate here already for $n'=8$, whereas for $kT_e=400$ eV the curves still deviate from the grid even at $n'=15$. This is due to the temperature dependence of the exponential factor, mentioned above, which appears in the expression of α^D_{kd} [see Eqs. (3) and (5)]. At low temperature however, the contribution of the high-lying complexes is very small, as shown in Figs. 1 and 2; therefore the error introduced into the total DR rate coefficients by an inaccurate extrapolation at low electron temperature is expected to be also very small. Finally, we have chosen the value of $n_s=9$. Consequently, the detailed level-by-level calculations have been performed for the partial DR rate coefficients along the Ni I sequence for all the complexes up to $n'=9$ only. Equation (7) can then be written as

$$\sum_{n'=4}^{\infty}\alpha^D(n')=\sum_{n'=4}^{9}\alpha^D(n')+4.028\alpha^D(9). \qquad (7')$$

In the Ta^{45+} case, the sum of the extrapolated contributions for all the $3d^94ln'l'$ ($n'>9$) complexes at $kT_e=400$ eV is only about 2% of the total DR rate coefficient, whereas at $kT_e=4$ keV it is approximately 18%.

It should be stressed that the present calculations have been carried out under the assumption of no inelastic electron-ion collisions after the initial electron capture. As the electron density increases, electron collisions become more important and are associated with a lowering of the continuum. These effects can severely affect the contributions of high-lying $3d^94ln'l'$ configurations to DR. In those cases the extrapolated contributions should be partially or even completely disregarded.

D. Total DR rate coefficients

After adding the sum of the extrapolated contributions of the $3d^94ln'l'$ ($n'>9$) configuration complexes to the contributions of the complexes calculated in Sec. III B, one finally obtains the *total* DR rate coefficients. These results are presented in Table III in the 10-eV to 10-keV electron temperature range for the ten Ni-like ions considered. The table also gives the calculated energy for the first ionization E_I(Cu) of the Cu-like ion in the ground state for each ion. Figure 4 shows the special behavior of the total DR rate coefficients for the various elements at low temperature. This effect is essentially due to the contributions of some particular levels close to the ionization limit in the $3d^94l4l'$ configuration complex, as discussed in Ref. [4].

Table IV shows the present total DR results for Gd^{36+} and Ta^{45+} compared to those obtained in Refs. [5, 6] using the multiconfiguration Dirac-Fock (MCDF) model, at various electron temperatures in the 50-eV to 3-keV range. We have found that in most cases the *partial* DR results of the present work are consistently about 20–30 % higher than those of the MCDF method at all electron temperatures. An unexplained exception is the factor 2 discrepancy in the partial rate coefficients for DR through the $3d^94l4l'$ complex of Gd, which has already been reported in Ref. [4]. Most of the discrepancies in the total DR rate coefficient for Gd at low temperatures in Table IV are due to the discrepancy for this

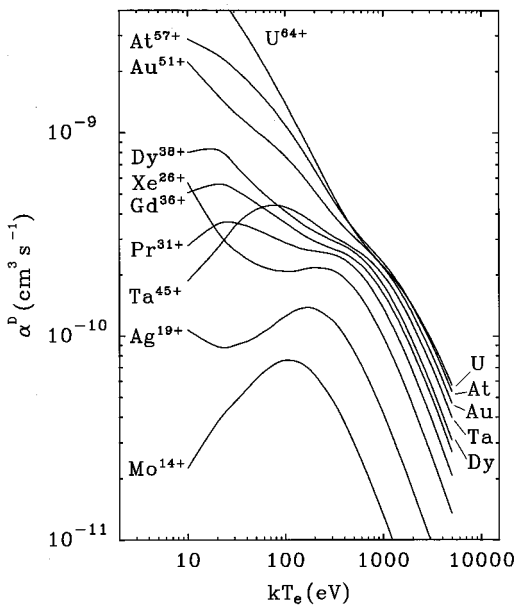

FIG. 4. Total DR rate coefficients for the ten Ni-like ions considered, as a function of the electron temperature.

TABLE IV. Total DR rate coefficients (in $cm^3\,s^{-1}$) for Gd^{36+} and Ta^{45+} at different electron temperatures, compared to the results of Ref. [5] (for Gd) and Ref. [6] (for Ta). $X[-Y]$ denotes $X\times10^{-Y}$.

		T_e (eV)				
Ion	Reference	50	100	300	1000	3000
Gd^{36+}	present work	4.51[−10]	3.61[−10]	2.70[−10]	1.62[−10]	5.26[−11]
	Ref. [5]	1.76[−10]	1.55[−10]	1.42[−10]	9.29[−11]	3.02[−11]
Ta^{45+}	present work	4.19[−10]	4.31[−10]	3.12[−10]	1.99[−10]	7.40[−11]
	Ref. [6]	3.27[−10]	3.56[−10]	2.52[−10]	1.48[−10]	5.46[−11]

complex that dominates the DR process at $kT_e<200$ eV. The residual discrepancies for both Gd and Ta at all temperatures are due to the present inclusion of NRS and DAC transitions that were neglected in Refs. [5, 6] and to the contributions of the high-lying $3d^9 4ln'l'$ ($n'>9$) configurations evaluated here by extrapolation, which were apparently neglected in Ref. [5] for Gd (but not in Ref. [6] for Ta).

In Fig. 5 the total DR rate coefficients obtained in the present work are compared to the results from the semiempirical Burgess-Merts (BM) approximation [8,9] for Mo^{14+}, Pr^{31+}, and U^{64+} in the 10-eV to 2.5-keV electron temperature range. Vertical dotted lines on the curves indicate for reference the temperature $kT_e=0.5E_I$(Cu) for each element. The predictions of this formula depend on the atomic data used in it. The results plotted in Fig. 5 have been obtained using the oscillator strengths and the transition energies computed by RELAC [11] for the strongest $3d$-$4f$ transition only, as suggested by Breton, De Michelis, and Mattioli [2]. At high electron temperature [$kT_e>0.5E_I$(Cu)], as shown in Fig. 5, the BM approximation *underestimates* the molybdenum DR rate coefficients by a factor of about 2. The results for praseodymium appear to be fairly good, whereas for uranium the BM approximation *overestimates* the DR coefficients by about 15%. The calculations show that the deviation of the BM curves for the other ions varies smoothly between the two extreme deviations for Mo and U. However, at low temperature [$kT_e<0.3E_I$(Cu)] the BM formula gives completely incorrect predictions for all the elements; it can underestimate the DR rate coefficients by up to a few orders of magnitude. Moreover, at low electron temperature the temperature dependence of the BM results is totally inadequate. The reasons for the inadequacy of the BM formula in the case of the isoelectronic sequence considered here are explained in the following.

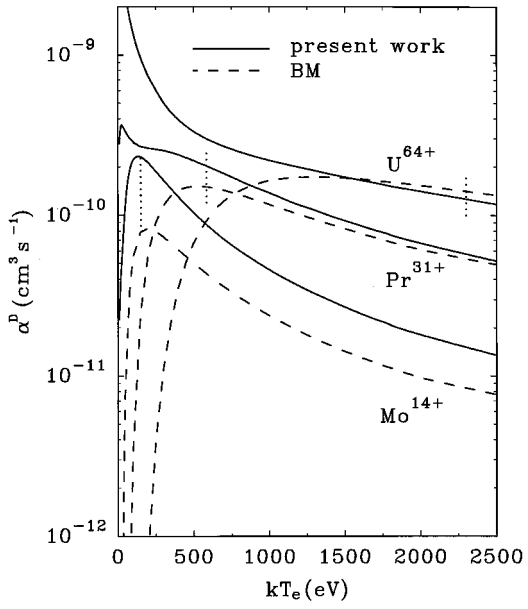

FIG. 5. Total DR rate coefficients for Mo^{14+}, Pr^{31+}, and U^{64+} as a function of the electron temperature. Solid curves show the results of the level-by-level calculations. Dashed curves indicate the results obtained from the Burgess-Merts (BM) formula. Vertical dotted lines on the curves indicate the temperature $kT_e=0.5E_I$(Cu) for each element.

Some substantial simplifying assumptions were made in the BM approximation. These assumptions are quite accurate for the weakly ionized atoms pertaining to sequences isoelectronic to light elements, but are no longer valid for the ions investigated here. The major simplification was to assume that the main contribution to DR comes from levels lying well above the ionization limit. Consequently, the exponential factor in Eq. (3) would be slowly varying from one individual level d to another and the energy term E_{kd} in the exponent could be substituted by an average energy constant term. In the present isoelectronic sequence, the $3d^9 4l4l'$ complex lies very close to the ionization limit and is the main contributor to DR at low electron temperature. In the case of Ni-like gadolinium, for instance, E_{kd} for this complex varies from 0 to 226 eV, making any constant approximation for the energy term in the exponent inadequate in the $0<kT_e<400$ eV range. Furthermore, the approximation that uses the energy and oscillator strength of the parent radiative transition (of the recombining ion) instead of the actual values (for the recombined ion) cannot be valid for levels so close to the ionization limit. In the Gd^{36+} case the BM approximation uses the average $3d^{10}$-$3d^9 4f$ transition energy of approximately 1420 eV, instead of the actual E_{kd} value (between 0 and 226 eV). Moreover, the calculations carried out by Burgess were performed for light elements in the nonrelativistic LS-coupling scheme. Thus the formula was originally stated to be valid only for ions of charge +20 at the most.

In conclusion, the Burgess-Merts formula cannot be expected to estimate the DR rate coefficients correctly for the heavy ions of the Ni I sequence at a low temperature. In this domain, not only are the magnitudes of the coefficients given by the formula inadequate, but so is the electron temperature behavior predicted by it. Therefore, accurate evaluation of

DR rate coefficients for ionized heavy elements in this temperature range necessitates detailed *ab initio* calculations.

IV. CONCLUSIONS

Detailed level-by-level calculations of the total DR rate coefficients for ground-state Ni-like ions have been performed and the results are presented for ten ions of the isoelectronic sequence. These results show that the nonresonant stabilizing radiative transitions can play an important role in the DR processes especially at very low electron temperature. On the other hand, the approximation that totally neglects decays to autoionizing levels is generally a sufficiently good one. The $3d^9 4l4l'$ inner-shell excited configuration complex has been found to give the main contribution to DR at low electron temperature due to the fact that the levels of this complex lie just above the ionization limit. At high temperature DR contributions of higher $3d^9 4ln'l'$ complexes become dominant, particularly the contribution of $3d^9 4l5l'$. The DR contributions of very high $3d^9 4ln'l'$ complexes have been found to scale as n'^{-3} already around $n'=9$, enabling an accurate extrapolation for the converging DR contributions of the complexes with $n'>9$. At high temperature these complexes contribute between 10% and 20% of the total DR rate coefficient.

It appears that the Burgess-Merts formula predicts the total DR rate coefficients with an accuracy better than $\pm 20\%$ for the heavy Ni-like ions ($Z>54$) at relatively high electron temperature [$kT_e > 0.5E_I$(Cu)]. However, at low temperature [$kT_e < 0.3E_I$Cu] it is completely inadequate; it can underestimate the total rate coefficients by up to a few orders of magnitude. In conclusion, the smooth temperature dependence of the DR rate coefficients at *high temperature* might make feasible the use of analytical approximations in this temperature range, as well as interpolation for other heavy Ni-like ions. However, in order to obtain correct DR rate coefficients at *low temperature* only detailed level-by-level calculations are adequate, due to the irregular behavior of the DR rate coefficients in this range. Thus, for accurate modeling of x-ray laser schemes and for determination of the precise fractional ion abundances in plasmas, such calculations are required. The results for the Ni I sequence may give an idea of the limitations expected from DR semiempirical approximations for neighboring sequences as well.

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