General analytic formula for total dielectronic recombination rate coefficients of Ni-like ions

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A general analytic formula for the total dielectronic recombination (DR) rate coefficients of all the ions along the NiI isoelectronic sequence with $34 \leqslant Z \leqslant 92$ is constructed on the basis of previously calculated DR data, which were obtained by relativistic *ab initio* level-by-level computations using the HULLAC code for ten Ni-like ions. The DR rate coefficients are given as a function of the electron temperature and of the ion charge. The results generated by this formula reproduce the previously calculated DR rate coefficients, generally to better than 5% accuracy for all electron temperatures $kT_e \geqslant 0.03E_I$ (E_I is the ionization energy of the Cu-like ion). As a test, the results of level-by-level DR calculations for two additional elements, barium and tungsten, are compared to those of the analytic formula. The agreement is found to be similar to that for the first ten ions. The analytic formula may be conveniently used for modeling the ion abundance distribution in hot plasmas. [S1050-2947(98)09009-X]

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I. INTRODUCTION

The importance of dielectronic recombination (DR) for calculating the ionization balance in hot plasmas is by now long recognized (e.g., Refs. [1–4]). However, due to the complexity of the calculations, the full effect of DR on highly ionized heavy atoms is still to be investigated. In particular, very few relativistic *ab initio* level-by-level DR calculations for highly ionized heavy ions isoelectronic to the third- and fourth-row elements have been published.

There are several published works on the DR of Ni-like ions. The total DR rate coefficients for Ni-like Gd and Ta in the ground state have been calculated in detail by Chen [5,6] using the multiconfiguration Dirac-Fock (MCDF) relativistic method [7]. Recently, the relativistic HULLAC (Hebrew University Lawrence Livermore Atomic Code) code developed by Bar-Shalom *et al.* [8] was used for a further systematic study of DR processes along the NiI isoelectronic sequence [9,10]. In a first study [9] we thoroughly investigated the DR of Ni-like ions in the ground state via the low-lying inner-shell excited $3d^9 4ln'l'$ ($n'=4,5$) Cu-like configurations. In the course of this study, the effect of *nonresonant radiative stabilizations* (NRS) and *decays* to *autoionizing* levels possibly followed by *cascades* (DAC) was analyzed. More recently, the results of the full calculations of the *total* DR rate coefficients for the Ni-like ions Mo^{14+}, Ag^{19+}, Xe^{26+}, Pr^{31+}, Gd^{36+}, Dy^{38+}, Ta^{45+}, Au^{51+}, At^{57+}, and U^{64+} in the ground state were presented [10]. These extensive level-by-level calculations include the DR contributions of the high-lying Cu-like configurations $3d^9 4ln'l'(n' \leqslant 9)$, $3p^5 3d^{10} 4ln'l'$ ($n' \leqslant 5$), and $3s3p^6 3d^{10} 4ln'l'$ ($n' \leqslant 5$) and take the effect of NRS and DAC transitions into account. The residual contributions of the even higher configurations were also accounted for using extrapolation methods. All the DR calculations for Ni-like ions were performed assuming no electron-ion collisions occur after the initial electron capture. A recent work using a collisional-radiative model [11] shows that for the low-lying DR channels this approximation is still valid for electron densities up to 10^{20} cm^{-3}. The total DR rate coefficients for Ni-like Gd and Ta obtained by the two different methods, MCDF and HULLAC, were compared [10] and found, for the most part, to agree within about 25% at most electron temperatures. These discrepancies have been mostly attributed to the inclusion of NRS and DAC transitions in the HULLAC calculations [10].

It was already found that the commonly used Burgess-Merts (BM) semiempirical formula [12,13], which was constructed for evaluating the total DR rate coefficients of low-Z ions, is not adequate for highly ionized heavy atoms in general, nor for the Ni-like ions in particular [5,10]. For the relatively light ($Z<50$) Ni-like ions, the BM approximation was found [10] to underestimate the DR rates by as much as a factor of 2. Moreover, at relatively low electron temperatures the BM approximation gives completely incorrect predictions for all the ions in the sequence [10]. In a completely different approach by Hahn [14], the contributions to the total DR rate coefficients are divided into five different excitation modes. However, this approximation is also designated for relatively light ($Z<50$) ions with only 12 electrons or fewer. Accordingly, the highest excitation mode included in this latter work is the $3s$ or $3p$ excitation, whereas the major mode for DR of Ni-like ions is the $3d$ excitation. In conclusion, no adequate approximation is available for the total DR rate coefficients of Ni-like ions or for ions in neighboring isoelectronic sequences.

In the present work, we seek to complete the investigation of the DR processes for Ni-like ions performed in Refs. [9] and [10] for ten elements only, by extending it to the rest of the NiI sequence. The main goal here is to construct a general expression for the *total* DR rate coefficients of all the elements along the NiI sequence, including those for which no level-by-level computations have been performed. On the basis of the extensive *ab initio* level-by-level calculations of the total DR rate coefficients performed for ten Ni-like ions in the 10 eV $\leqslant kT_e \leqslant$ 10 keV electron temperature range [10], one shows that a simple approximate analytic function of the electron temperature and of the ion charge can indeed be derived. This approximation enables an evaluation of the total DR rate coefficients for all the Ni-like ions from Se^{6+} to U^{64+}. This task is not straightforward because of the highly irregular DR contributions from ion to ion of the $3d^9 4l4l'$ Cu-like levels, which along the sequence move from above

the ionization limit to below it [9]. It has been shown that a single level that lies just above the ionization limit may completely dominate the DR processes at low electron temperatures. Moreover, this irregular behavior, which is reflected in the total DR rate coefficients mostly at low temperatures, may still have repercussions at high temperatures.

The present analytic formula is useful for reproducing the results of the total DR rate coefficients calculated in Ref. [10], but it is mostly aimed at giving the total DR rate coefficients for the other Ni-like ions with an accuracy of the same order of the level-by-level calculations (believed to be about 10%) in the electron temperature range for which the ion abundances in most of the plasmas may be significant. Finally, the accuracy of the analytic formula is assessed here by comparison to new *ab initio* level-by-level DR calculations carried out for two other ions, Ni-like Ba^{28+} and W^{46+}.

II. THEORETICAL METHOD

In the following a very brief outline of the methods for calculating the DR rate coefficients is given. The total rate coefficient for dielectronic recombination of the recombining (Ni-like) ion in an initial state k is obtained by summing over all the DR channels, i.e., all intermediate inner-shell excited levels d of the recombined (Cu-like) ion:

$$\alpha_k^D = \sum_d \beta_{kd} B^D(d), \tag{1}$$

where β_{kd} is the rate coefficient for dielectronic capture from level k to level d and $B^D(d)$ is the probability for effective recombination by radiative stabilization after the initial capture, i.e., the *branching ratio for DR through level d* [10]. In the Ni-like case, for instance, it was found that in order to obtain accurate results, the sum in Eq. (1) should be taken over more than 17 000 levels d [10]. An analytic approximate formula may open the possibility to avoid these very complex and time-consuming DR calculations for ions that have not yet been investigated.

Since β_{kd} has the following dependence on kT_e:

$$\beta_{kd} \approx (kT_e)^{-1.5} \exp\left(\frac{-E_{kd}}{kT_e}\right), \tag{2}$$

E_{kd} being the energy difference between levels k and d, the straightforward approach is to try to estimate α_k^D by a parametric sum expression of the type

$$\alpha_k^D = (T_e)^{-1.5} \sum_{i=1}^{m} A_i \exp(-B_i/T_e). \tag{3}$$

This method was already proposed by Burgess in 1965 [12] and by Roszman in 1987 [15]. According to Burgess, the summation in Eq. (3) should be over each of the numerous relevant stabilizing transitions. Roszman suggested a limited summation over five ($m=5$) exponential terms: two for the $\Delta n=0$ transitions and three for the $\Delta n>0$ transitions. We have tested several alternative analytic functions, but have found that expression (3) with m taken to be 3 gives the best results for DR in the NiI sequence where there are $\Delta n>0$ transitions only. After fitting the parameters A_i and B_i to best reproduce the existing DR data, the second step is to fit these parameters to functions of the ion charge r.

Instead of using kT_e in the parametric sum expression [Eq. (3)], it is more convenient to define a reduced electron temperature τ in units of the ionization energy E_I for each recombined (Cu-like) ion:

$$\tau = \frac{kT_e}{E_I}. \tag{4}$$

Thus, the general analytic expression for the DR rate coefficients of Ni-like ions proposed here is

$$\alpha_k^D = (\tau)^{-1.5}[\exp(A_1 - B_1/\tau) + \exp(A_2 - B_2/\tau) + \exp(A_3 - B_3/\tau)]. \tag{5}$$

The choice of three exponential terms (in square brackets) appears indeed to be the most adequate. It enables us to best introduce the different DR effects due to 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 ($B_1<B_2<B_3$). It should be noted that expression (5) includes only six parameters. In order to reflect the ion charge dependence of α_k^D, each parameter is in turn represented by a function of the ion charge r. Unlike in previous works for other sequences [16], in the present work these functions are simple four-term power series of r, which are shown to satisfactorily reproduce all the DR results.

III. RESULTS

A. Accurate parameters for reproducing the detailed DR calculations

As a first step, following the method described in the preceding section, the level-by-level DR computation results for the ten ions of Ref. [10] are fitted to expression (5). The best-fit procedure is performed for each ion separately in order to obtain the six parameters for each one. The values of these parameters are presented in Table I. By using these parameters in expression (5) it is possible to reproduce the total DR rate coefficients with an accuracy as good as about 2% for temperatures $kT_e \geqslant 0.03E_I$, which cover the whole domain in which the ions may exist with a significant abundance in most plasmas. It should be noted that an accuracy of 2% is much better than the intrinsic accuracy of the level-by-level HULLAC calculations, which is expected to be of the order of 10%. Consequently, the analytic function formula can be conveniently used for the DR rate coefficients of these ten ions for modeling the ionization states in plasmas.

B. Interpolated parameters for the whole NiI sequence

As a second step, we evaluate the parameters in expression (5) for all the remaining ions in the NiI sequence as described in the following. In order for the analytic formula [expression (5)] to be adequate for as many Ni-like ions as possible, we first extend the basic results of Ref. [10], in which Mo ($Z=42$) is the lightest element investigated, by

TABLE I. Parameters obtained by a best-fit procedure of expression (5) to the total DR rate coefficients of ten Ni-like ions calculated by detailed level-by-level computations in Ref. [10]. $X[-Y]$ stands for $X\times10^{-Y}$.

Ion	A_1	B_1	A_2	B_2	A_3	B_3
Mo^{14+}	−27.232	8.0288[−2]	−24.876	0.29630	−23.221	0.82488
Ag^{19+}	−26.931	4.2276[−2]	−24.424	0.26278	−22.692	0.77839
Xe^{26+}	−26.301	2.7619[−2]	−24.192	0.21398	−22.455	0.71011
Pr^{31+}	−25.967	3.2754[−2]	−24.268	0.17748	−22.462	0.66127
Gd^{36+}	−25.876	2.7414[−2]	−24.281	0.16690	−22.590	0.63417
Dy^{38+}	−25.727	2.6647[−2]	−24.133	0.17914	−22.636	0.63001
Ta^{45+}	−25.529	3.9629[−2]	−24.375	0.16497	−22.815	0.58865
Au^{51+}	−25.564	2.1549[−2]	−24.586	0.12238	−22.978	0.54260
At^{57+}	−25.682	1.3465[−2]	−24.873	8.9869[−2]	−23.108	0.50055
U^{64+}	−25.752	9.2056[−3]	−25.179	9.1348[−2]	−23.324	0.47616

calculating the DR rate coefficient of an even lighter element. For this purpose the Ni-like Kr^{8+} ($Z=36$) ion has been selected. For much lower charged ions the HULLAC code based on the parametric potential method is not accurate enough. *Ab initio* level-by-level calculations are performed here for Kr^{8+}, but only for DR through the relatively low-lying Cu-like $3d^9 4l n'l'$ ($n'=4,5$) configuration complexes. These DR channels are the dominant channels at most electron temperatures [10]. The *total* DR rate coefficient for Kr^{8+} is subsequently evaluated by assuming that the relative contribution of these DR channels to the total DR rate coefficient at each electron temperature in the Kr case is roughly the same as for Mo, for which both partial [9] and total [10] DR rate coefficients were previously calculated in detail. From these approximate results for the total DR rate coefficient of Kr^{8+} the best-fit parameters A_i and B_i are obtained for this ion as well.

Subsequently, the values of each of the six parameters for the previously investigated ten ions (Table I) and for Kr^{8+} are fitted to six corresponding r-dependent power series. Unlike in other works (e.g., Ref. [16]), here series of a small number of r-dependent terms are found to be sufficient. The parameters are fitted to six series of only four r^x terms, selected in such a way that they still reproduce the original parameter values previously obtained for the eleven ions with a satisfactory accuracy. The limited number of r^x terms (here four) is intended to best insure the accuracy of the interpolation for the DR rate coefficients of the intermediate ions not previously calculated. This procedure leads to the following expressions for the various parameters:

$$A_1=25.116r^{-1}-31.792+0.225\,10r-2.1852\times10^{-3}r^2, \tag{6a}$$

$$B_1=1.3572r^{-1}-6.1320\times10^{-2}+2.2979\times10^{-3}r-2.3559\times10^{-5}r^2, \tag{6b}$$

$$A_2=-27.018+0.29041r-4.5091\times10^{-3}r^2+2.6027\times10^{-5}r^3, \tag{6c}$$

$$B_2=29.556r^{-2}-2.7263r^{-1}+0.400\,75-4.5993\times10^{-3}r, \tag{6d}$$

$$A_3=-37.562r^{-1}-19.739-5.3608\times10^{-2}r+1.0164\times10^{-4}r^2, \tag{6e}$$

and

$$B_3=102.06r^{-2}-11.431r^{-1}+1.2593-1.0259\times10^{-2}r. \tag{6f}$$

Using these functions for the parameters in expression (5), the total DR rate coefficients for any Ni-like ion can be easily obtained. The coefficients generated using the analytic formula [expression (5) and Eqs. (6a)–(6f)] for all the Ni-like ions from Se ($Z=34$) to U ($Z=92$) are given in Table II for electron temperatures kT_e equal to $0.1E_I$, $0.3E_I$, E_I, $3E_I$, and $10E_I$. The calculated ionization energies E_I are given in the second column of the table. For the ten elements investigated in Ref. [10] and for Ba and W (see the next section), the total DR rate coefficients obtained by level-by-level calculations are also given in the table below the results generated by the analytic formula. It should be stressed that if any analytic expression is desired for the DR total rate coefficients of these ions (for modeling purposes), it is preferable to use in expression (5) the directly fitted parameters given in Table I, instead of those deduced from Eqs. (6a)–(6f), in order to achieve higher accuracy.

As can be seen from Table II, the discrepancies between the level-by-level calculated data [10] and those obtained by the general analytic formula [expression (5) and Eqs. (6a)–(6f)] in the $0.1E_I \leqslant kT_e \leqslant 10E_I$ electron temperature range are generally found to be less than 10%, and in most of the cases less than 5%. The discrepancies increase at low temperatures and are in fact inherent in any method of interpolation between ions along the sequence, due to the highly irregular variations from ion to ion of the DR contributions of the low-lying Cu-like $3d^9 4l 4l'$ configuration complex, since more levels (important to DR) of these configurations fall below the ionization limit as Z increases [9]. Although the higher-lying complexes give rather smooth contributions to the total DR rate coefficients, the $3d^9 4l 4l'$ irregularities still have a residual effect at high temperatures as well. This effect is most pronounced for Ni-like Ta, for which the total DR rate coefficients at low temperatures are particularly small with respect to the general trend along the sequence

TABLE II. Total DR rate coefficients (in $cm^3\,s^{-1}$) for Ni-like Se^{6+} to Ni-like U^{64+} obtained by using the general analytic formula [expression (5) and Eqs. (6a)–(6f)] for various electron temperatures in units of the ionization energy E_I of the Cu-like ion. Superscripts ''a'' and ''b'' indicate the results of the detailed level-by-level computations. $X[-Y]$ stands for $X\times10^{-Y}$.

		kT_e				
Ion	E_I (eV)	$0.1E_I$	$0.3E_I$	$1.0E_I$	$3.0E_I$	$10.0E_I$
Se^{6+}	80.67	1.97[−11]	1.52[−11]	6.15[−12]	1.85[−12]	3.72[−13]
Br^{7+}	101.6	1.83[−11]	1.50[−11]	7.41[−12]	2.44[−12]	5.01[−13]
Kr^{8+}	124.4	1.90[−11]	1.78[−11]	1.05[−11]	3.55[−12]	7.28[−13]
Rb^{9+}	149.2	2.13[−11]	2.30[−11]	1.52[−11]	5.09[−12]	1.03[−12]
Sr^{10+}	175.9	2.51[−11]	3.06[−11]	2.12[−11]	6.98[−12]	1.40[−12]
Y^{11+}	204.3	3.00[−11]	4.03[−11]	2.82[−11]	9.09[−12]	1.80[−12]
Zr^{12+}	234.8	3.61[−11]	5.16[−11]	3.58[−11]	1.13[−11]	2.23[−12]
Nb^{13+}	266.9	4.31[−11]	6.41[−11]	4.37[−11]	1.36[−11]	2.66[−12]
Mo^{14+}	301.1	5.09[−11]	7.72[−11]	5.16[−11]	1.59[−11]	3.08[−12]
		4.72[−11]a	7.51[−11]a	4.87[−11]a	1.50[−11]a	2.93[−12]a
Tc^{15+}	337.0	5.94[−11]	9.05[−11]	5.93[−11]	1.80[−11]	3.49[−12]
Ru^{16+}	374.8	6.87[−11]	1.04[−10]	6.66[−11]	2.01[−11]	3.87[−12]
Rh^{17+}	414.4	7.86[−11]	1.17[−10]	7.35[−11]	2.20[−11]	4.23[−12]
Pd^{18+}	455.9	8.91[−11]	1.29[−10]	7.99[−11]	2.37[−11]	4.56[−12]
Ag^{19+}	499.3	1.00[−10]	1.41[−10]	8.57[−11]	2.53[−11]	4.85[−12]
		9.89[−11]a	1.37[−10]a	8.46[−11]a	2.54[−11]a	4.94[−12]a
Cd^{20+}	545.3	1.12[−10]	1.53[−10]	9.10[−11]	2.67[−11]	5.11[−12]
In^{21+}	591.8	1.24[−10]	1.64[−10]	9.57[−11]	2.80[−11]	5.34[−12]
Sn^{22+}	640.8	1.36[−10]	1.74[−10]	9.99[−11]	2.90[−11]	5.53[−12]
Sb^{23+}	691.4	1.49[−10]	1.84[−10]	1.04[−10]	3.00[−11]	5.70[−12]
Te^{24+}	744.4	1.62[−10]	1.93[−10]	1.07[−10]	3.07[−11]	5.84[−12]
I^{25+}	799.4	1.76[−10]	2.01[−10]	1.10[−10]	3.14[−11]	5.95[−12]
Xe^{26+}	855.7	1.90[−10]	2.09[−10]	1.12[−10]	3.19[−11]	6.04[−12]
		2.09[−10]a	2.13[−10]a	1.15[−10]a	3.51[−11]a	6.33[−12]a
Cs^{27+}	915.0	2.04[−10]	2.16[−10]	1.14[−10]	3.23[−11]	6.10[−12]
Ba^{28+}	974.6	2.18[−10]	2.23[−10]	1.15[−10]	3.25[−11]	6.14[−12]
		2.15[−10]b	2.24[−10]b	1.17[−10]b	3.49[−11]b	6.32[−12]b
La^{29+}	1037	2.32[−10]	2.29[−10]	1.16[−10]	3.27[−11]	6.16[−12]
Ce^{30+}	1102	2.46[−10]	2.34[−10]	1.17[−10]	3.27[−11]	6.16[−12]
Pr^{31+}	1168	2.60[−10]	2.39[−10]	1.17[−10]	3.27[−11]	6.15[−12]
		2.80[−10]a	2.45[−10]a	1.19[−10]a	3.44[−11]a	
Nd^{32+}	1237	2.74[−10]	2.43[−10]	1.18[−10]	3.26[−11]	6.12[−12]
Pm^{33+}	1307	2.87[−10]	2.47[−10]	1.17[−10]	3.24[−11]	6.07[−12]
Sm^{34+}	1379	3.00[−10]	2.50[−10]	1.17[−10]	3.22[−11]	6.01[−12]
Eu^{35+}	1454	3.13[−10]	2.52[−10]	1.16[−10]	3.18[−11]	5.95[−12]
Gd^{36+}	1531	3.25[−10]	2.54[−10]	1.16[−10]	3.15[−11]	5.87[−12]
		3.14[−10]a	2.46[−10]a	1.12[−10]a	3.18[−11]a	
Tb^{37+}	1609	3.37[−10]	2.56[−10]	1.15[−10]	3.11[−11]	5.78[−12]
Dy^{38+}	1691	3.48[−10]	2.57[−10]	1.13[−10]	3.06[−11]	5.69[−12]
		3.43[−10]a	2.58[−10]a	1.13[−10]a	3.04[−11]a	
Ho^{39+}	1772	3.59[−10]	2.57[−10]	1.12[−10]	3.01[−11]	5.59[−12]
Er^{40+}	1858	3.68[−10]	2.57[−10]	1.10[−10]	2.96[−11]	5.48[−12]
Tm^{41+}	1944	3.77[−10]	2.57[−10]	1.09[−10]	2.90[−11]	5.37[−12]
Yb^{42+}	2034	3.85[−10]	2.56[−10]	1.07[−10]	2.84[−11]	5.25[−12]
Lu^{43+}	2125	3.93[−10]	2.55[−10]	1.05[−10]	2.78[−11]	5.14[−12]
Hf^{44+}	2219	3.99[−10]	2.54[−10]	1.03[−10]	2.72[−11]	5.02[−12]
Ta^{45+}	2315	4.04[−10]	2.52[−10]	1.01[−10]	2.66[−11]	4.89[−12]
		3.43[−10]a	2.41[−10]a	1.01[−10]a	2.58[−11]a	
W^{46+}	2414	4.09[−10]	2.50[−10]	9.94[−11]	2.60[−11]	4.77[−12]
		3.55[−10]b	2.36[−10]b	9.55[−11]b	2.48[−11]b	4.78[−12]b

TABLE II. (*Continued*).

Ion	E_I (eV)	kT_e				
		$0.1E_I$	$0.3E_I$	$1.0E_I$	$3.0E_I$	$10.0E_I$
Re^{47+}	2514	4.12[−10]	2.47[−10]	9.73[−11]	2.53[−11]	4.64[−12]
Os^{48+}	2616	4.14[−10]	2.44[−10]	9.52[−11]	2.47[−11]	4.52[−12]
Ir^{49+}	2722	4.16[−10]	2.42[−10]	9.31[−11]	2.40[−11]	4.40[−12]
Pt^{50+}	2829	4.16[−10]	2.38[−10]	9.09[−11]	2.34[−11]	4.27[−12]
Au^{51+}	2939	4.15[−10]	2.35[−10]	8.87[−11]	2.27[−11]	4.15[−12]
		4.09[−10][a]	2.35[−10][a]	8.86[−11][a]	2.30[−11][a]	
Hg^{52+}	3052	4.14[−10]	2.31[−10]	8.66[−11]	2.21[−11]	4.03[−12]
Tl^{53+}	3166	4.12[−10]	2.28[−10]	8.44[−11]	2.15[−11]	3.90[−12]
Pb^{54+}	3283	4.08[−10]	2.24[−10]	8.22[−11]	2.08[−11]	3.78[−12]
Bi^{55+}	3403	4.04[−10]	2.20[−10]	8.01[−11]	2.02[−11]	3.67[−12]
Po^{56+}	3525	4.00[−10]	2.16[−10]	7.79[−11]	1.96[−11]	3.55[−12]
At^{57+}	3650	3.94[−10]	2.12[−10]	7.58[−11]	1.90[−11]	3.44[−12]
		4.19[−10][a]	2.17[−10][a]	7.84[−11][a]		
Rn^{58+}	3778	3.89[−10]	2.07[−10]	7.37[−11]	1.84[−11]	3.33[−12]
Fr^{59+}	3908	3.82[−10]	2.03[−10]	7.16[−11]	1.78[−11]	3.22[−12]
Ra^{60+}	4041	3.75[−10]	1.99[−10]	6.96[−11]	1.73[−11]	3.11[−12]
Ac^{61+}	4177	3.68[−10]	1.95[−10]	6.76[−11]	1.67[−11]	3.01[−12]
Th^{62+}	4315	3.61[−10]	1.91[−10]	6.57[−11]	1.62[−11]	2.91[−12]
Pa^{63+}	4456	3.53[−10]	1.87[−10]	6.38[−11]	1.57[−11]	2.81[−12]
		3.46[−10]	1.83[−10]	6.19[−11]	1.51[−11]	2.71[−12]
U^{64+}	4601	3.57[−10][a]	1.83[−10][a]	6.39[−11][a]		

[a]Detailed calculations in Ref. [10].
[b]Detailed calculations in Ref. [17].

[10] due to the *small* contribution of the $3d^9 4l4l'$ complex, as shown in Ref. [9]. As a result, the general formula, which follows the mean trend of the sequence, *overestimates* the actual DR rate coefficients for Ni-like Ta by up to 18% at $kT_e = 0.1E_I$ and by still 3% at $kT_e = 3E_I$. Another example for the effect of the $3d^9 4l4l'$ irregularities is the Ni-like Xe ion. However, in contrast to the Ta case, in the Xe case the $3d^9 4l4l'$ complex has several strong DR channels via levels lying just above the ionization limit, giving a particularly *large* contribution to the total DR rate coefficients [9]. As a result, the general formula *underestimates* the actual DR rate coefficients for Ni-like Xe by almost 10% at $kT_e = 0.1E_I$ and by still 5% at $kT_e = 10E_I$. For the other Ni-like ions, the discrepancies between the general formula and the level-by-level calculations at low electron temperatures ($kT_e < 0.1E_I$) are smaller. It should be noted that for all ions at *very low* electron temperatures ($kT_e < 0.005E_I$) the results of the analytic formula *underestimate* the DR rate coefficients with respect to the accurately computed values. The precise DR rates at these temperatures can be obtained by detailed level-by-level calculations only. It should be noted, however, that at very low temperatures the DR rates may be sensitive to the plasma environment, for example, to electric field effects. Consequently, even the results of the detailed DR calculations for these temperatures should be used with caution.

Figure 1 shows as an illustration the DR rate coefficients for Ni-like Ag and Au obtained by the different methods: the level-by-level calculations [10], the analytic formula [expression (5)] using the accurate parameters (from Table I), the general analytic formula [also expression (5) but with Eqs. (6a)–(6f) instead of the accurate parameters], and finally the BM approximation [12,13]. It can be seen that the general analytic formula gives accurate results down to electron temperatures as low as $0.02E_I$, and with the accurate parameters the results are practically the same as those obtained by the detailed calculations in the electron temperature range considered. On the other hand, the BM approximation is no longer adequate already at $kT_e \leqslant 0.3E_I$. At high electron temperatures, the BM approximation gives an overestimation of about 25% for Ag and 10% for Au, while the general analytic formula reflects the detailed calculations very well. The results for Ag and Au shown in the figure are representative of the other ions throughout the sequence. Therefore, Fig. 1 can give an idea of the typical accuracy expected from the present formula [both when using Eqs. (6a)–(6f) and when using the parameters in Table I] and from the BM approximation, for all Ni-like ions.

Although the fitting of the parameters A_i and B_i to the data is carried out for ions only as light as Kr, the results obtained by using the analytic formula for the next two lighter elements Br and Se are still expected to be sufficiently accurate and are also given in Table II. Extrapolation to lighter elements beyond Se is unreliable.

IV. LEVEL-BY-LEVEL CALCULATIONS FOR Ni-LIKE Ba AND W

In order to assess the accuracy of the analytically generated DR rate coefficients for all the Ni-like ions, extensive level-by-level DR calculations were performed for two additional Ni-like ions, Ba^{28+} and W^{46+}, which were not included in Ref. [10] and thus not used for obtaining Eqs. (6a)–(6f).

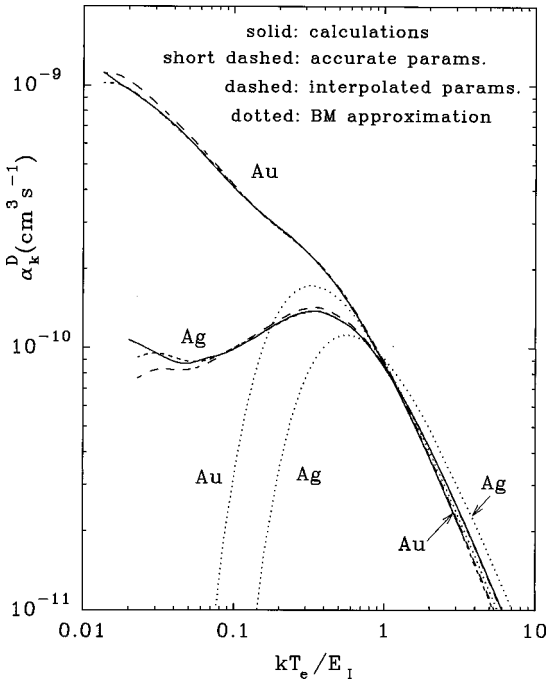

FIG. 1. Total DR rate coefficients for Ag^{19+} and Au^{51+} as a function of the electron temperature in reduced units of the ionization energy E_I of the Cu-like ion. The solid curves show the results of the level-by-level calculations (Ref. [10]). The short-dashed curves represent the results of the analytic formula [expression (5)] using the accurate parameters in Table I. The dashed curves represent the results of the general analytic formula [expression (5) and Eqs. (6a)–(6f)]. The dotted curves give the Burgess-Merts (BM) approximation.

The computation procedure is identical to the one employed in Ref. [10]. The details of the computations for Ba and W, including the partial contributions of the various configuration complexes, are published elsewhere [17]. Here, only the final results of the *total* DR rate coefficients for these ions are given in Table II and denoted by the superscript ''b'' for comparison with the values obtained by using the general analytic formula. It can be clearly seen that the agreement is quite good: For Ba the discrepancies are less than 3%, whereas for W the agreement is very good at high temperatures and the discrepancy increases to about 15% at low temperatures. The relatively large discrepancy for W^{46+} at low temperatures is due to the same effect as for the Ta^{45+} ion discussed in the preceding section, i.e., a particularly small DR contribution of the $3d^9 4l 4l'$ complex. This effect is characteristic of the Cu-like ions of the elements around $Z=73$, for which the autoionizing $3d^9 4l 4l'$ levels are not very close to the ionization limit.

V. CONCLUSION

The lack of accurate DR data for most of the Ni-like ions has motivated us to develop a general analytic expression for evaluating the total DR rate coefficients along the NiI sequence ($34 \leqslant Z \leqslant 92$). These data are necessary for modeling the fractional ion abundances of heavy elements in plasmas. The present work saves the tedious task of level-by-level DR calculations for the Ni-like ions not yet investigated. The proposed formula is constructed on the basis of previous detailed DR calculations for ten ions along the NiI sequence. The total DR rate coefficients are given for all the Ni-like ions as a function of the electron temperature and the ion charge. The results generated by the analytic formula in the $0.1E_I < kT_e < 10E_I$ electron temperature range are found to reproduce the previously calculated data to generally better than 5%. At lower temperatures ($0.01E_I < kT_e < 0.1E_I$) the results generated by the analytic formula are usually still accurate to about 15%. The formula is also checked by comparison with *new* level-by-level calculations performed independently for the DR rate coefficients of Ni-like Ba and W. The formula is found to reproduce these DR rate coefficients with the same accuracy. In the absence of accurate DR data for isoelectronic sequences adjacent to NiI, the present analytic formula with minor corrections to include the $\Delta n = 0$ transitions should be appropriate for ionization balance modeling in these other sequences as well.

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[1] A. Burgess, Astrophys. J. **139**, 776 (1964).
[2] M. Arnaud and R. Rothenflug, Astron. Astrophys., Suppl. Ser. **60**, 425 (1985).
[3] C. Breton, C. De Michelis, and M. Mattioli, J. Quant. Spectrosc. Radiat. Transf. **19**, 367 (1978).
[4] K. B. Fournier, M. Cohen, W. H. Goldstein, A. L. Osterheld, M. Finkenthal, M. J. May, J. L. Terry, M. A. Graf, and J. Rice, Phys. Rev. A **54**, 3870 (1996).
[5] M. H. Chen, Phys. Rev. A **35**, 4129 (1987).
[6] M. H. Chen, Phys. Rev. A **47**, 4775 (1993).
[7] I. P. Grant, *et al.*, Comput. Phys. Commun. **21**, 207 (1980); B. J. Mckenzie, *et al.*, *ibid.* **21**, 233 (1980).
[8] A. Bar-Shalom, M. Klapisch, and W. H. Goldstein, the HULLAC code for atomic physics, 1988 (unpublished).
[9] E. Behar, P. Mandelbaum, J. L. Schwob, A. Bar-Shalom, J. Oreg, and W. H. Goldstein, Phys. Rev. A **52**, 3770 (1995).
[10] E. Behar, P. Mandelbaum, J. L. Schwob, A. Bar-Shalom, J. Oreg, and W. H. Goldstein, Phys. Rev. A **54**, 3070 (1996).
[11] E. Behar, A. Peleg, R. Doron, P. Mandelbaum, and J. L. Schwob, J. Quant. Spectrosc. Radiat. Transf. **58**, 449 (1997).
[12] A. Burgess, Astrophys. J. **141**, 1588 (1965).
[13] A. L. Merts, R. D. Cowan, and N. H. Magee, Jr., Los Alamos Scientific Laboratory Report No. LA-6220-MS, Los Alamos, New Mexico, 1976 (unpublished).
[14] Y. Hahn, J. Quant. Spectrosc. Radiat. Transf. **49**, 81 (1993).
[15] L. J. Roszman, Phys. Rev. A **35**, 2122 (1987).
[16] H. Teng, B. Sheng, W. Zhang, and Z. Xu, Phys. Scr. **49**, 463 (1994).
[17] E. Behar, P. Mandelbaum, and J. L. Schwob (unpublished).