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Theoretical transition probabilities and lifetimes in nickel–like Se^{6+}, Y^{11+} and Sn^{22+} ions

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Abstract. The 17 levels of the $3d^{10}$, $3d^9 4s$ and $3d^9 4p$ configurations, and the electric–dipole transitions among these levels are calculated for the three nickel–like ions Se^{6+}, Y^{11+} and Sn^{22+} by using large–scale multiconfiguration Dirac–Fock wavefunctions. From these computations, the excitation energies and transition probabilities as well as the lifetimes of $3d^9 4p$ levels are derived, including all dominant effects of relativity, correlation and of the rearrangement of the electron density within the same framework. Comparison is made with the scarce number of experimental data and previous semi–empirical computations.

PACS. 32.70.Cs Oscillator strengths, lifetimes, transition moments

1 Introduction

The shell structure of the nickel–like ions are known to offer unique possibilities for a coherent amplification in the EUV and soft X–ray domain. When compared with the more frequently studied neon isoelectronic sequence, a much higher amplification is usually achieved owing to the (open and near–by lying) $3d$ and $4f$ shells. Moreover, the level structure of the nickel–like ions ensures that the so–called *water–window* at 23.2–43.7 Å is reached already at a moderate degree of ionization. Therefore, the transitions among the low–lying levels of the nickel–like ions have attracted a lot of recent interest, both by experiment and computations [1–17]; see also reference [18] for a recent review on this topic. Apart from potential X–ray laser applications, several of the electric–dipole allowed and *forbidden* lines from the nickel sequence were found useful also in the diagnostics of high–temperature plasmas as they arise, for example, in the interaction of intense optical laser pulses with matter, vacuum sparcs or in tokamak devices.

So far, however, most experiments on the nickel–like ions focused on the identification of a few strong transitions and only to a much smaller extent onto a detailed measurement of branching fractions, lifetimes, or transition probabilities. While, for instance, (i) the $3d^9 4p$–$3d^9 4s$ and $3d^9 4d$–$3d^9 4p$ electric–dipole (E1) transitions were observed and classified already earlier for the ions near the neutral end of the sequence [1–6], later work mainly focused on (ii) the strong dipole lines from the $3d^9 4p$–$3d^{10}$ and $3d^9 4f$–$3d^{10}$ configurations in various highly–charged ions [7] as well as (iii) on the identification of *forbidden* electric–quadrupole (E2) transitions between the $3d^9 4s$–$3d^{10}$ and $3p^5 3d^{10} 4f$–$3d^{10}$ configurations [8], or (iv) even on electric– (E3) and magnetic–octupole (M3) lines [9], which arise between the $3d^{10}$ ground and a few excited states. In recent years, moreover, the wavelengths (or levels) of a few possible $3d^9 4d$–$3d^9 4p$ *laser lines* have been identified for several highly–charged ions in the nickel isoelectronic sequence [10,11].

By far less emphasis has been paid to the measurement of transition probabilities and lifetimes which have been carried out only for the spectrum of Cu II [16,17]. Of course, several theoretical investigations along the nickel sequence are available today which, however, were often based on rather limited computations such as the modified distorted–wave calculations of Zhang *et al.* [12], who generated oscillator strengths for all the 33 nickel–like ions in the range $60 \leq Z \leq 92$, or the multiconfiguration Dirac–Fock (MCDF) computations by Quinet and Biémont [13] for the highly charged ions Ag^{19+} to Pb^{54+} and Biémont [14] for selected ions in the range Sn^{22+} to U^{64+}, who both studied the electric–dipole allowed and several forbidden transitions among the 17 levels of the low–lying $3d^{10}$, $3d^9 4s$ and $3d^9 4p$ configurations. In these multiconfiguration calculations, however, a rather small configuration basis was used and the relaxation effects on the electron density omitted completely. In addition, Loginov [15] made use of a least–square procedure and statistical arguments in order to estimate the transition probabilities and lifetimes for the nickel–like ions Cu^+ to Mo^{14+}. Such a least–square procedure may work well for predicting the excitation and transition energies along an isoelectronic sequence but carries some risk for deriving probabilities

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and lifetimes which, usually, appear much more sensitive to near–lying levels (of the same symmetry) or even to the occurrence of level crossings.

In the following, we report on an elaborate computation of the 17 levels from the $3d^{10}$, $3d^9 4s$ and $3d^9 4p$ configurations, and the electric–dipole *allowed* (E1) transitions among these levels. Systematically enlarged MCDF calculations have been carried out for the three multiple–charged ions Se^{6+}, Y^{11+}, and Sn^{22+} in the intermediate Z region of the nickel isoelectronic sequence where the effects of relativity, correlation, and of the rearrangement of the electron density need to be treated consistently within the same framework. From these computations, the intensity ratios and lifetimes of all 12 levels of the $3d^9 4p$ configuration are derived. The present investigation continues our recent work on the Cu II [19], where a wave function expansion of similar extent was used to resolve the long–standing "puzzle" on the intensity and transition probability of the $3d^9 4p\ ^1\mathrm{P}_1^o - 3d^{10}\ ^1\mathrm{S}_0$ resonance line. Comparison of our theoretical results is made with the scarce number of experimental data and the (semi–empirical) computations by Biémont [14] and Loginov [15].

2 Theoretical method

To generate the wavefunctions of the low–lying levels, we utilized the two atomic structure packages GRASP92 [20] and RATIP [21] which implement the MCDF method and which have been designed explicitly for large–scale computations on open–shell atoms and ions. Since, however, this method has been explained in many papers before (see, for example, the review by Grant [22]), we only give a very brief account here. In the multiconfiguration Dirac–Fock method, an atomic state is approximated by a linear combination of configuration state functions (CSF) of the same symmetry

$$\psi_\alpha(PJM) = \sum_{r=1}^{n_c} c_r(\alpha)\, |\gamma_r PJM\rangle\,, \qquad (1)$$

where n_c is the number of CSF, which characterizes the size of the wavefunction expansion. In the GRASP92 program, each CSF is built from antisymmetrized products of a common set of *orthonormal* Dirac orbitals which are represented on a numerical grid. Both, the radial orbital functions *and* the expansion coefficients $\{c_r(\alpha),\ r = 1, \ldots, n_c\}$ are optimized self–consistently on the basis of the Dirac–Coulomb Hamiltonian. Further relativistic corrections from (transverse) Breit interactions among the electrons are added later to the Hamiltonian matrix as a perturbation from which the complete wavefunction expansion, *i.e.* the representation $\{c_r(\alpha)\}$ in (1), is finally obtained by diagonalization. Although some programs are available today, where the self–consistent field can be based on the Dirac–Coulomb–Breit Hamiltonian [23], a perturbative treatment of the Breit interaction appears to us justified for the study of valence–shell transitions and, typically, introduces uncertainties which are negligible when compared with missing correlations [24]. In addition, QED corrections have been also estimated from the wave functions above by making use of a simple model due to Kim [25] and it's implementation into the RELCI [26] component of the RATIP program. These radiative corrections are negligible for the Se^{6+} ions but were incorporated into the transition energies of the Y^{11+} and Sn^{22+} ions.

In practise, different MCDF computations often need to be distinguished due to the size of the wave function expansions which are utilized, *i.e.* the number n_c of CSF in (1), reflecting the extent to which electron–electron correlations are taken into account. While earlier computations were usually restricted to just a few (tens of) CSF, nowadays, wave function expansions of several ten thousand CSF are easily applicable due to the recent developments of the atomic structure codes [20,21]. However, such *sizeable* wave functions are also necessary in order to obtain a sufficiently accurate description of the level structure and transition properties of open–shell ions. In the study of several valence–shell structures along different isoelectronic sequences we found, for instance, that virtual excitations of electrons from the (spectroscopically) occupied shells into the subshells of the *next two (unoccupied) layers* are typically needed to obtain accurate transition probabilities, at least for the strong and medium transitions [24,27–29]. For some of the weak lines, in fact, an even larger effort may become necessary [30].

3 Computational procedure

For the nickel–like ions, the low–lying level structure consists of the $3d^{10}\ ^1\mathrm{S}_0$ ground state, the four levels of the $3d^9 4s$ with total angular momenta $J = 1$, 2, and 3, as well as the 12 upper, odd–parity levels with total angular momenta $J = 0$, ..., 4 which arise from the $3d^9 4p$ configuration. Thus, dipole–allowed (E1) transitions only occur between these upper levels and the levels with proper angular momenta from the $3d^{10}$ and $3d^9 4s$ configurations; of course, these E1 *allowed* transitions also govern the lifetimes of the $3d^9 4p$ levels since the dipole–forbidden M1 and E2 transitions (among the levels of the same parity) are usually smaller by several orders of magnitudes. In carrying out large–scale computations, one can benefit to a great deal from exploiting the symmetries of the atomic levels as the Hamiltonian matrix is diagonal in the total angular momenta J and parity P. Therefore, a natural start position for our computations was to divide the levels into 9 level groups and to carry out an independent optimization procedure for each of the symmetries J^P. But although this procedure enables one to incorporate *relaxation effects* in the electron density directly into the wavefunction representation (1), an independent optimization also yields orbital functions for each level group which are not quite orthogonal to the orbitals of any other group and, hence, requires additional effort in the computation of the transition matrix elements as discussed below. In practise, such an approach is equivalent to the use of a *no–pair* Hamiltonian which, however, is based on a "multiconfigurational potential". Although this neglects the influence from the negative energy states,

Table 1. Number of CSF in the wave function expansion for the various level groups and for different computational models.

Configuration	J^P	SC	4SD	5SD
$3d^{10}$	0^+	1	1016	5821
$3d^9 4s$	1^+	1	915	5024
	2^+	2	1334	7364
	3^+	1	1446	8288
$3d^9 4p$	0^-	1	674	4198
	1^-	3	1876	11806
	2^-	4	2687	17262
	3^-	3	2997	19837
	4^-	1	2830	19533

this approach has been found sufficient for the study of E1 allowed transitions. For the magnetic–dipole (M1) *forbidden* transitions, in contrast, rather large contributions from the negative energy states have been found recently for helium–like ions [31] as well as for the alkali atoms [32].

Apart from the use of the Dirac–Hamiltonian for representing the (kinetic) energy of each single electron, *electron–electron correlations* certainly play the most essential role in studying the low–lying excitation spectrum of (many–electron) atoms and ions. In multiconfiguration calculations, these correlations are treated most properly by (some type of) the *active space method*, although often at the price of rather large expansions. In the present study, a series of computations have been carried out by including electron–electron correlations within different computational models and by monitoring, how the excitation energies and transition probabilities (begin to) converge. Table 1 lists the numbers of CSF which were used in the wave function expansions of the various level groups and in the different models. Beside the single configuration (SC) model, which basically displays the number of the spectroscopically considered levels in each group, we also treated several enlarged expansions where we incorporated all single and double excitations of the $3d$, $4s$, and $4p$ electrons into the $4s$, $4p$, $4d$, and $4f$ subshells (hereafter referred to as the 4SD approximation, including excitations within the $4l$ layer) as well as, in addition, into the $4s$, ..., $5f$ shells (5SD). For these two approximations, finally, independent computations have been carried out for each level group. To obtain our final results below, we made use of the wave function expansions from the last column (5SD) in which, for the odd–parity levels, up to about 20,000 CSF were taken into account.

In studying *transition arrays*, some part of the electron–electron correlation is treated very efficiently by carrying out an independent *variation* of the initial and final state wavefunctions. In the past, therefore, different techniques have been developed in order to incorporate these *relaxation effects* on the electron density also in the computation of the transition matrix [30,33–36]. In the RATIP package, we exploit a determinant expansion of the atomic wave functions and the expressions of Löwdin [33], by making use of the two (new) components CESD99 [37] and REOS99 [38] within the RATIP code. These two components are now appropriate also for large wavefunction expansions (up to several ten thousand CSF) and already helped improve the available data base for various ions along different isoelectronic sequences [24,27–29]. Moreover, the incorporation of relaxation effects into the transition matrix typically brings the (length and velocity) gauge forms closer together and, overall, leads to quite improved transition probabilities.

4 Results and discussions

4.1 Excitation energies of the $3d^9 4s$ and $3d^9 4p$ levels from the ground state

Excitation energies and E1 transition probabilities have been calculated for the 17 levels from the $3d^{10}$, $3d^9 4s$ and $3d^9 4p$ configurations. They are presented below for the three multiple–charged ions Se^{6+}, Y^{11+} and Sn^{22+} in the intermediate Z range of the nickel isoelectronic sequence. Table 2 shows the excitation energies of the $3d^9 4s$ and $3d^9 4p$ levels relative to the (closed–shell $3d^{10}$) $^1S_0$ ground state. In this table, a level number and the overall symmetry (J^P) is assigned to each level which are used below to denote the individual transitions. While, however, these level numbers are defined in ascending energy order for the Se^{6+} ion, this order is not quite correct for the levels $8 \ldots 15$ of the Y^{11+} and Sn^{22+} ions due to the appearance of a few level crossings at a higher stage of ionization. Overall, good agreement is found with the (few) experimentally available energies and the semi–empirical extrapolations [4], whereby a – nearly constant – shift of the $3d^9 4s$ and $3d^9 4p$ excitation energies towards higher values indicate that the more stable (and closed–shell) $^1S_0$ ground–state is slightly better represented within the given configuration basis. This shift amounts to about 1500 cm^{-1} for the Se^{6+} ion and increases to approximately 4000 cm^{-1} for Sn^{22+}.

A shift of the excitation energies (of the low–lying levels) towards higher values is generally expected for all multiple–charged ions, but occurs in contrast to the theoretical energies which we obtained recently — within the same wavefunction expansion — for the single–ionized Cu^+ ion [19]. For this ion, the theoretical energies slightly *underrate* the observed excitation energies. To understand this different behaviour at the neutral end of the isoelectronic sequence in more detail, we carried out a number of additional calculations by including various (classes of) excitations into the $4l$ and $5l$ layers. From these computations, we found that triple excitations into the $3d$ and $4l$ orbitals (*i.e.* within an 4SDT approximation) do not influence much the total energies of the multiple–charged ions, neither for the ground–state nor for the excited levels, but lower considerably the $3d^{10}$ and $3d^9 4s$ level energies of the single–ionized ion and, hence, should be incorporated in the computations for Cu^+. For higher charge states, of course, both triple excitations as well as the excitations

Table 2. Excitation energies (in cm^{-1}) of the 17 levels of the $3d^{10}$, $3d^9 4s$ and $3d^9 4p$ configurations in Se^{6+}, Y^{11+} and Sn^{22+} ions.

Label		Se^{6+}		Y^{11+}		Sn^{22+}	
No.	J^P	This work	Exp. [4]	This work	Calc. [6]	This work	Calc. [6]
1	0^+	0	0	0	0	0	0
2	3^+	441372	439749	1148886	1146688	3592573	3591029
3	2^+	443763	442116	1152843	1150631	3599786	3598319
4	1^+	448300	446765	1165943	1163838	3664286	3662742
5	2^+	451811	450303	1170046	1168099	3669774	3668594
6	2^-	560859	558702	1343505	1339342	3957969	3951852
7	3^-	565376	563615	1348963	1345518	3963928	3959041
8	1^-	567795	565640	1362504	1358253[a]	4040120	4034698[b]
9	4^-	569734	568118	1365087	1361441	4054641	4050006
10	2^-	570216	568536	1362584	1359354	4030309	4025571
11	0^-	571582	569777	1374501	1370434	4113464	4107205
12	2^-	576893	575110	1374375	1370699	4066260	4061399
13	3^-	577177	575552	1377145	1373654	4075382	4071219
14	3^-	579958	578370	1386353	1383239	4132804	4128902
15	1^-	580052	578270	1378323	1374873[a]	4070376	4065041[b]
16	1^-	583112	581485	1390234	1386905[a]	4135259	4130354[b]
17	2^-	584375	582753	1393396	1390213	4144279	4140379

[a] Experiment by Wyart *et al.* [2,3]; [b] experiment by Burkhalter *et al.* [1].

into the $5l$ layer become less important and can be neglected from the wave function expansions. For the Sn^{22+} ions, therefore, we expect our excitation energies to be accurate to about $\lesssim 0.1\%$.

4.2 The $3d^9 4p - 3d^{10}$ and $3d^9 4p - 3d^9 4s$ transition probabilities

Tables 3–5 display the wavelengths and transition probabilities of all (allowed) E1 transitions of the $3d^9 4p - 3d^{10}$ and $3d^9 4p - 3d^9 4s$ configurations, given in an ascending order of the transition energies. As mentioned before, the individual transitions are specified by the level numbers of the corresponding upper and lower states; moreover, the transition probabilities are listed in two gauge forms, *i.e.* in length and velocity gauge (respectively, Babushkin and Coulomb gauge in a relativistic notation), in order to provide an indication of the quality of the data as well as reference for further investigations. Of course, an agreement of the different gauge forms for any individual line does not say much about the accuracy of these data, but the overall agreement (or disagreement) for a whole transition array certainly provides some insight into the quality of the approximation. Note, moreover, that the inclusion of negative energy states might be required in order to obtain full gauge invariance [31,32]. Usually, however, the length–gauge results are considered to be more reliable since they "probe" the wave functions in a similar (radial) region as the *variation procedure* does for the total level energies. Apart from the transition probabilities, we also list the weighted oscillator strengths (in length gauge) for the emission from the upper level as well as the results from previous computations.

Good agreement between the probabilities in lengths and velocity gauge is obtained for the strong and for most of the medium lines. But although all transitions are *caused* by the coupling of the radiation field to the electronic motion of the ion, the weaker lines often appear more sensitive to electron–electron correlations and, hence, much larger deviations among the different gauge forms may occur for these lines. In Tables 3–5 below, the two gauges typically agree within about 10% for the strong and medium lines which often becomes better even if the nuclear charge increases along the isoelectronic sequence. For the two ions Se^{6+} and Y^{11+}, however, a few exceptions arise for example for the lines 6–2 and 11–4, for which the length and velocity gauge *disagrees* by more than 20%. For these two lines, we found that the probabilities still vary rather much in going from the 4SD to the 5SD wave functions and, thus, seem not (yet) to be "converged" with regard to the size of the wave function expansion. A very similar situation was found also for several of the weak line, such as the transitions 6–5 and 10–2 for the Se^{6+} ion which, however, are suppressed by $3 \ldots 4$ orders of magnitude when compared with the strong resonance lines of this ion. These transitions have to be considered as "intercombination" lines where often large cancellations occurs for the transition amplitudes.

In Tables 3 and 4, comparison of our transition probabilities for the Se^{6+} and Y^{11+} ions is made with the estimates of Loginov [15] who applied statistical arguments and a least–square procedure on a set of experimental and semiempirical energies. Although such a procedure may help improve (some of) the excitation energies, if a

Table 3. Theoretical wavelengths λ, transition probabilities A, and oscillator strengths gf for the $3d^9 4p - 3d^{10}$ and $3d^9 4p - 3d^9 4s$ E1 dipole transitions of Se^{6+} ion. The level numbers of the transitions in the first column refer to Table 2. The numbers in brackets denote powers of ten.

	λ (Å)	A (s^{-1})			
Transition	This work	Length	Velocity	Loginov [15]	gf
6−5	917.03	4.38(7)	6.02(7)	4.69(7)	2.76(−2)
6−4	888.43	7.84(6)	1.03(7)	7.65(6)	4.64(−3)
7−5	880.54	5.35(7)	5.35(7)	6.02(7)	4.35(−2)
8−5	862.19	3.21(8)	4.02(8)	3.58(8)	1.07(−1)
6−3	853.99	2.14(7)	4.50(7)	2.12(7)	1.17(−2)
10−5	844.55	2.14(8)	1.98(8)	2.41(8)	1.14(−1)
6−2	836.92	2.37(9)	2.94(9)	2.62(9)	1.24
8−4	836.87	2.35(8)	3.31(8)	2.47(8)	7.40(−2)
7−3	822.27	1.85(9)	1.61(9)	2.06(9)	1.31
6−4	820.24	1.60(9)	1.38(9)	1.78(9)	8.10(−1)
11−4	811.15	2.72(9)	3.36(9)	3.00(9)	2.69(−1)
8−3	806.25	2.13(9)	2.55(9)	2.32(9)	6.24(−1)
7−2	806.42	6.78(8)	6.30(8)	8.01(8)	4.63(−1)
12−5	799.47	6.68(8)	6.67(8)	7.44(8)	3.20(−1)
13−5	797.66	1.13(9)	1.09(9)	1.14(9)	7.59(−1)
10−3	790.80	8.23(8)	7.58(8)	9.63(8)	3.85(−1)
15−5	779.78	2.30(9)	2.45(9)	2.52(9)	6.29(−1)
9−2	779.19	3.01(9)	2.68(9)	3.41(9)	2.47
14−5	780.36	1.72(9)	1.55(9)	3.01(9)	1.10
12−4	777.65	3.76(8)	3.58(8)	4.55(8)	1.70(−1)
10−2	776.13	6.02(6)	3.26(6)	8.73(6)	2.72(−3)
16−5	761.61	3.16(8)	3.76(8)	3.97(8)	8.26(−2)
15−4	759.01	5.83(8)	5.73(8)	7.55(8)	1.51(−1)
17−5	754.35	2.13(9)	2.11(9)	2.44(9)	9.09(−1)
12−3	751.14	2.11(9)	2.12(9)	2.39(9)	8.95(−1)
13−3	749.55	3.06(8)	2.95(8)	4.13(8)	1.80(−1)
16−4	741.78	2.48(9)	2.47(9)	2.77(9)	6.15(−1)
12−2	737.89	5.10(6)	3.96(6)	1.63(6)	2.08(−4)
13−2	736.35	1.76(9)	1.70(9)	2.15(9)	1.00
17−4	734.89	8.91(8)	8.31(8)	1.02(9)	3.60(−1)
14−3	734.24	6.81(8)	6.13(8)	7.35(8)	3.85(−1)
15−3	733.73	1.96(8)	2.32(8)	1.96(8)	4.75(−2)
14−2	721.58	8.61(8)	8.68(8)	8.85(8)	4.70(−1)
16−3	717.62	6.78(8)	6.26(8)	8.21(8)	1.57(−1)
17−3	711.17	2.63(8)	2.58(8)	3.02(8)	1.00(−1)
17−2	699.29	1.22(8)	1.02(8)	1.49(8)	4.50(−2)
8−1	176.12	3.05(8)	2.91(8)	2.70(8)	4.26(−3)
15−1	172.40	3.53(10)	3.45(10)	3.39(10)	4.72(−1)
16−1	171.49	1.00(10)	9.86(9)	1.13(10)	1.33(−1)

particular trend is known for the uncertainties along the isoelectronic sequence, we have doubts how reliable this method works for predicting transition probabilities. For the resonance line 14–5 of the Se^{6+} ions, for instance, we found a rather stable value of $\sim 1.7 \times 10^9$ within both, our 4SD and 5SD approximations, while Loginov predicts a value of 3.0×10^9 which is larger by almost a factor of 2. A similar case has been found for the strong line 12–5 of the Y^{11+} ions with a deviation of more than 50% while the two gauge forms from our computations agree within about 3%. For the weak lines, moreover, deviations up to a factor of 10 are found in this comparison which can be traced back to an insufficient configuration basis as used in Loginov's earlier computations.

For the Sn^{22+} ions with a much higher nuclear charge, Table 5 compares our transition probabilities with previous MCDF results by Biémont [14]. Here, a rather good

Table 4. Theoretical wavelengths λ, transition probabilities A, and oscillator strengths gf for the $3d^9 4p - 3d^{10}$ and $3d^9 4p - 3d^9 4s$ E1 dipole transitions of Y^{11+} ion. The level numbers of the transitions in the first column refer to Table 2. The numbers in brackets denote powers of ten.

	λ (Å)	A (s^{-1})			
Transition	This work	Length	Velocity	Loginov [15]	gf
6−5	577.29	8.63(7)	1.35(8)	9.22(8)	2.15(–2)
6−4	563.93	1.24(7)	1.59(7)	1.14(7)	2.96(–3)
7−5	559.66	3.17(7)	3.64(7)	3.85(7)	1.04(–2)
6−3	525.14	4.01(7)	2.12(7)	4.19(7)	8.29(–3)
8−5	520.23	1.77(9)	2.18(9)	1.91(9)	2.15(–1)
10−5	520.01	1.16(9)	1.11(9)	1.27(9)	2.35(–1)
6−2	514.43	5.47(9)	6.79(9)	5.95(9)	1.08
7−3	510.51	3.89(9)	3.40(9)	4.28(9)	1.06
8−4	509.36	1.38(8)	2.69(8)	1.46(8)	1.61(–2)
10−4	509.15	3.28(9)	2.82(9)	3.60(9)	6.38(–1)
8−3	500.38	1.89(9)	1.77(9)	2.16(9)	4.98(–1)
12−5	489.97	8.42(8)	8.26(8)	1.27(9)	1.51(–1)
13−5	483.41	5.78(8)	5.01(8)	6.05(8)	1.41(–1)
15−5	480.67	4.11(9)	4.37(9)	4.52(9)	4.28(–1)
12−4	480.31	6.89(8)	6.73(8)	8.17(8)	1.19(–1)
11−4	480.02	7.05(9)	8.77(9)	7.60(9)	2.43(–1)
8−3	477.50	4.68(9)	5.60(9)	5.04(9)	4.80(–1)
10−3	477.32	1.52(9)	1.43(9)	1.77(9)	2.60(–1)
15−4	471.37	1.31(9)	1.35(9)	1.59(9)	1.31(–1)
10−2	468.45	2.74(6)	1.53(6)	9.40(5)	4.50(–4)
9−2	463.02	7.73(9)	6.88(9)	8.56(9)	2.23
14−5	462.81	7.04(9)	6.38(9)	7.80(9)	1.58
16−5	454.64	6.68(8)	8.52(8)	7.55(8)	6.21(–2)
12−3	451.88	6.23(9)	6.41(9)	6.86(9)	9.54(–1)
17−5	448.20	5.34(9)	5.40(9)	5.97(9)	8.04(–1)
16−4	446.31	6.77(9)	6.93(9)	7.45(9)	6.06(–1)
13−3	446.30	2.32(9)	2.18(9)	2.62(9)	4.85(–1)
15−3	443.97	1.95(9)	2.24(9)	2.03(9)	1.73(–1)
12−2	443.93	1.39(8)	2.31(8)	1.23(8)	2.05(–2)
17−4	440.10	2.94(9)	2.77(9)	3.28(9)	4.28(–1)
13−2	438.54	5.73(9)	5.63(9)	6.51(9)	1.15
14−3	428.69	5.30(8)	4.73(8)	5.85(8)	1.02(–1)
16−3	421.67	1.25(9)	1.12(9)	1.54(9)	1.00(–1)
14−2	421.52	3.57(8)	3.88(8)	3.94(8)	6.66(–2)
17−3	416.12	1.86(8)	1.93(8)	2.21(8)	2.41(–2)
17−2	409.36	1.82(8)	1.35(8)	2.27(8)	2.28(–2)
8−1	73.394	2.44(8)	2.35(8)	2.49(8)	5.92(–4)
15−1	72.552	1.95(11)	1.92(11)	1.75(11)	4.62(–1)
16−1	71.930	4.49(10)	4.44(10)	4.65(10)	1.04(–1)

agreement is found, although Biémont applied a quite restricted configuration basis and provided data only for the strong (resonance) lines with $A > 10^9$ s^{-1}. In this comparison, the largest deviation of about 22% occurs for the resonance lines 15–1 and, again, can be traced back to the neglect of relaxation effects (which lower the probabilities by about 15%) and the rather limited set of configurations in Biémont's computations. In his investigation, in fact, configuration interactions were incorporated only among the four (nonrelativistic) configurations $3d^{10} + 3d^9 4s + 3d^9 4d + 3d^8 4s^2$ for all the $3d^{10}$ and $3d^9 4s$ even–parity levels and among just the three configurations $3d^9 4p + 3d^9 4f + 3d^9 4s 4p$ for the upper, odd–parity levels. Today, such a limited configuration basis might be still appropriate for highly–charged ions (the main emphasis of Biémont's work [14]) but seems insufficient for

Table 5. Theoretical wavelengths λ, transition probabilities A, and oscillator strengths gf for the $3d^9 4p - 3d^{10}$ and $3d^9 4p - 3d^9 4s$ E1 dipole transitions of Sn^{22+} ion. The level numbers of the transitions in the first column refer to Table 2. The numbers in brackets denote powers of ten.

	λ (Å)	A (s^{-1})			
Transition	This work	Length	Velocity	Biémont [14]	gf
6−5	346.98	5.49(7)	1.20(8)		4.05(–3)
6−4	340.50	8.68(6)	1.05(7)		7.54(–4)
7−5	339.95	5.42(6)	1.19(7)		6.58(–4)
6−3	279.18	1.43(9)	1.16(9)	1.33(9)	8.40(–2)
10−5	277.36	5.78(9)	5.72(9)	5.77(9)	3.33(–1)
7−3	274.62	9.25(9)	8.21(9)	9.54(9)	7.32(–1)
6−2	273.67	1.36(10)	1.68(10)	1.42(10)	7.68(–1)
10−4	273.20	8.29(9)	7.20(9)	8.57(9)	4.64(–1)
8−5	270.01	1.18(10)	1.39(10)	1.18(10)	3.89(–1)
7−2	269.28	6.14(9)	5.86(9)	6.18(9)	4.67(–1)
8−4	266.07	6.87(8)	4.07(8)		2.18(–2)
12−5	252.21	6.04(8)	5.39(8)		2.88(–2)
15−5	249.62	3.00(9)	2.96(9)		8.41(–2)
12−4	248.77	6.63(8)	7.09(8)		3.07(–2)
13−5	246.54	1.74(8)	1.39(8)		1.11(–2)
15−4	246.25	1.96(9)	2.34(9)		5.34(–2)
10−3	232.27	1.53(9)	1.42(9)		6.21(–2)
10−2	228.44	9.87(7)	2.04(8)		3.86(–3)
8−3	227.10	5.70(9)	6.68(9)	6.67(9)	1.32(–1)
11−4	222.62	2.91(10)	3.56(10)	3.02(10)	2.16(–1)
9−2	216.41	3.14(10)	2.85(10)	3.23(10)	1.98
14−5	215.96	3.13(10)	2.89(10)	3.19(10)	1.53
15−5	214.82	3.50(9)	4.59(9)	3.69(9)	7.26(–2)
12−3	214.37	2.68(10)	2.78(10)	2.72(10)	9.23(–1)
15−3	212.50	2.53(10)	2.85(10)	2.51(10)	5.15(–1)
16−4	212.32	2.84(10)	2.98(10)	2.87(10)	5.76(–1)
12−2	211.11	3.58(9)	4.79(9)	3.60(9)	1.19(–1)
17−5	210.74	1.90(10)	1.95(10)	1.93(10)	6.34(–1)
13−3	210.26	1.30(10)	1.23(10)	1.32(10)	6.06(–1)
17−4	208.33	1.49(10)	1.42(10)	1.51(10)	4.87(–1)
13−2	207.12	2.14(10)	2.12(10)	2.16(10)	9.63(–1)
14−3	187.61	2.89(8)	2.51(8)		1.07(–2)
16−3	186.75	1.52(9)	1.13(9)		2.39(–2)
14−2	185.10	1.22(8)	1.68(8)		4.41(–3)
17−3	183.65	6.66(7)	8.40(7)		1.68(–3)
17−2	181.25	2.06(8)	1.01(8)		5.08(–3)
8−1	24.751	1.53(11)	1.53(11)	1.48(11)	4.21(–2)
15−1	24.567	1.38(12)	1.38(12)	1.68(12)	3.76(–1)
16−1	24.182	2.08(11)	2.08(11)	2.01(11)	5.48(–2)

all lower charge states or even near the neutral end of the isoelectronic sequence. Despite of the moderate influence of configuration interactions on the strong lines, an enlarged CSF basis such as our 4SD or 5SD is certainly required in studying medium and weak transitions of single and multiple ionized ions.

Since, unfortunately, (almost) no experimental data are yet available for the intermediate Z range of the nickel sequence, the accuracy of our theoretical predictions is less simple to estimate. From a detailed analysis of several multiple–charged ions along the chlorine isoelectronic sequence [24,27], we found that virtual excitations into the *next two unoccupied layers* and a level (group) independent generation of the wave functions improves the accuracy in the transition probabilities to about 10–15% for most strong and medium lines. In addition, by performing similar computations for Cu^+ ions [19], we were recently able to provide much better theoretical data for the intensity of the $^1P_1^o - {}^1S_0$ resonance line which resolved a "puzzling deviation" from the last few years. Again,

Table 6. Lifetimes (in 10^{-12} s) of the $3d^9 4p$ levels for Se^{6+}, Y^{11+} and Sn^{22+} ions.

	Se^{6+}			Y^{11+}			Sn^{22+}		
Level	Length	Velocity	Loginov [15]	Length	Velocity	Loginov [15]	Length	Velocity	Biémont [14]
6	408.56	326.51	370.24	182.82	147.27	163.90	66.31	55.68	64.39
7	386.49	435.52	341.42	173.01	193.42	154.40	64.98	71.07	63.61
8	333.51	279.42	312.10	146.41	120.92	136.10	5.84	5.75	5.99
9	331.58	373.13	292.59	129.37	145.35	116.80	31.85	35.09	30.96
10	377.20	426.09	333.49	167.50	186.57	150.68	64.52	69.93	69.74
11	366.45	297.54	332.55	141.84	114.03	131.59	34.36	28.09	33.11
12	315.75	316.86	278.40	126.58	122.85	114.19	31.57	29.41	32.47
13	311.95	323.65	269.40	115.87	120.34	102.77	29.07	29.85	28.74
14	306.06	329.23	270.00	126.10	138.12	113.90	31.95	34.60	31.35
15	26.01	26.46	26.71	4.94	5.00	5.46	0.76	0.71	0.59
16	73.79	74.97	65.00	18.66	18.76	17.80	4.15	4.12	4.29
17	293.26	301.93	255.58	115.61	117.65	103.10	29.50	29.67	29.07

wavefunction expansion of appropriate size and the incorporation of relaxation effects into the evaluation of the transition matrix were found to be the *key features* which are necessary in order to bring the theoretical predictions in agreement with experiment.

4.3 Lifetimes of the 3d^{9}4p levels

Finally, Table 6 shows the lifetimes of the 12 upper $3d^9 4p$ levels which we derived from the transition probabilities. Since, basically, the lifetime of a level reflects its most strongest decay branches, it often appears less sensitive to correlation effects, at least if the considered level can decay via one or several E1 allowed transitions. Again, our theoretical results are displayed in length and velocity gauge in order to facilitate further investigations. When compared with Loginov's semi–empirical estimates [15], our lifetimes are generally larger by about 10 ... 15%, apart from the very short–living level 15. For Sn^{22+}, however, our results are in reasonable agreement with the lifetimes of Biémont [14] as derived from his transition probabilities for the strong resonance lines.

As usual, all lifetimes decrease (rapidly) as the nuclear charge is increased along the isoelectronic sequence. This follows directly from the increase of the transition energies and a corresponding decrease of the radial extent of the wave functions. Deviations from this *simple rule* are sometimes observed, however, within a small range of Z values, if a level crossing nearby or strong configuration interactions enhance or reduce the transition probability of the main resonance line considerably. For the $3d^9 4p$ configuration, a rather remarkable decrease in the lifetimes occurs, in particular, for the three $J = 1$ levels 8, 15, and 16 due to the rapid growth of the $\Delta n = 1$ transition probabilities for their decay into the $^1S_0$ ground state. In fact, the short lifetimes of the $J = 1$ levels allows for a *population inversion* between the $3d^9 4p$ and $3d^9 4d$ levels and, hence, a spontaneous amplification in the X–ray regime. For the $3d^9 4d$–$3d^9 4p$ laser lines, a laser saturation has first been demonstrated recently for the three nickel–like ions Pd^{18+}, Ag^{19+} and Sn^{22+} by using a low–power pump mechanism [39].

5 Conclusions

Theoretical excitation energies and transition probabilities have been calculated for the 17 levels of the $3d^{10}$, $3d^9 4s$, and $3d^9 4p$ configurations, by applying large–scale multiconfiguration Dirac–Fock wavefunctions. Results are presented and compared with a small number of experimental data and previous (semi–empirical) computations for the three nickel–like ions Se^{6+}, Y^{11+} and Sn^{22+}. From the E1 transition probabilities of the $3d^9 4p$–$3d^{10}$ and $3d^9 4p$–$3d^9 4s$ transitions, the lifetimes of the 12 upper, odd–parity levels are derived; this study therefore extends our previous computations on the resonance and intercombination lines of the Cu^+ ion towards intermediate Z–values, where the effects of relativity, correlation and of the rearrangement of the electron density still need to be treated on the same footing. This requirement is seen, in particular, for the lifetimes of the Se^{6+} and Y^{11+} ions which are found larger by more than 10% when compared with earlier, semi–empirical computations by Loginov [15]. For higher values of Z, in contrast, the relativistic effects become dominant and, then, may allow to *reduce* some of the computational effort [14]. With our systematically enlarged wave functions, however, we are able to provide consistent and improved data not only for the (strong) resonance lines but also for the medium and weak transitions.

In recent years, the rapid growth in the available computer power has made the use of systematically enlarged wave function expansions possible, with which the *convergence* of atomic properties can be observed. However, apart from the much bigger size of now feasible wavefunction expansions, the continuous effort in developing efficient structure code appears (to us) of quite similar importance. With the RATIP package [21], we now provide a powerful environment for studying (relativistic) atomic transition and ionization properties, including Auger and photoionization properties. For a detailed analysis of optical and EUV spectra, hereby the inclusion

of the rearrangement effects of the electron density as a standard technique [38] was a major step to predict accurate transition probabilities also for multiple and highly charged ions.

With the present case study and the compilation of all E1 allowed transitions, we also hope to stimulate further experiments on multiple–charged ions for which spectroscopic information is needed not only in astro and plasma physics but also in a number of recently emerging fields such as UV– and X–ray lithographie, the generation of nanostructures, or the development of table–top X–ray laser. During the last years, accurate measurements on multiple charged ions became manageable mainly due to the developments on electron–beam ion traps (EBIT's) [40,41] and the operation of heavy–ion storage rings [42]. To further improve also the theoretical data base on the nickel–like ions, core–core correlations from the inner $3s$ and $3p$ subshells may have to be treated which were not included in the present computations. Until now, however, the systematic incorporation of core correlations is a less (well) understood topic in MCDF computations and, overall, for most open–shell structures.

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References

1. P.G. Burkhalter, U. Feldman, R.D. Cowan, J. Opt. Soc. Am. **64**, 1058 (1974)
2. J.–F. Wyart, J. Reader, A.N. Ryabtsev, J. Opt. Soc. Am. **71**, 692 (1981)
3. J.–F. Wyart, T.A.M. van Kleef, A.N. Ryabtsev, Y.N. Joshi, Phys. Scripta **29**, 319 (1984)
4. T.A.M. van Kleef, Y.N. Joshi, J. Opt. Soc. Am. **67**, 472 (1977); J. Opt. Soc. Am. B **1**, 271 (1984)
5. J.–F. Wyart, A.N. Ryabtsev, Phys. Scripta **33**, 215 (1986)
6. J.–F. Wyart, Phys. Scripta **36**, 234 (1987)
7. N. Tragin, J.–P. Geindre, P. Monier, J.–C. Gauthier, C. Chenais–Popovics, J.–F. Wyart, C. Bauche–Arnoult, Phys. Scripta **37**, 72 (1988)
8. J.–F. Wyart, C. Bauche–Arnoult, J.–C. Gauthier, J.–P. Geindre, P. Monier, M. Klapisch, A. Bar–Shalom, A. Cohn, Phys. Rev. A **34**, 701 (1986)
9. P. Beiersdorfer, A.L. Osterheld, J. Scofield, B. Wargelin, R.E. Marrs, Phys. Rev. Lett. **67**, 2272 (1991)
10. J.H. Scofield, B.J. MacGowan, Phys. Scripta **46**, 361 (1992)
11. Y. Li, J. Nilsen, J. Dunn, A.L. Osterheld, A. Ryabtsev, S. Churilov, Phys. Rev. A **58**, R2668 (1998)
12. H.L. Zhang, D.H. Sampson, C.J. Fontes, At. Data Nucl. Data Tables **48**, 91 (1991)
13. P. Quinet, E. Biémont, Phys. Scripta **43**, 150 (1991)
14. E. Biémont, J. Phys. B **30**, 4207 (1997)
15. A.V. Loginov, Phys. Scripta **47**, 38 (1993)
16. J.R. Crespo Lopez–Urruti, B. Kenner, T. Neger, H. Jäger, J. Quant. Spectrosc. Radiat. Transfer **52**, 111 (1994)
17. E.H. Pinnington, G. Rieger, J.A. Kernahan, E. Biémont, Can. J. Phys. **75**, 1 (1997)
18. H. Daido *et al.*, Int. J. Mod. Phys. B **11**, 945 (1997)
19. C.Z. Dong, S. Fritzsche, B. Fricke, J. Elec. Spec. Rel. Phenom **114–116**, 157 (2001)
20. F.A. Parpia, C. Froese Fischer, I.P. Grant, Compt. Phys. Commun. **94**, 249 (1996)
21. S. Fritzsche, J. Elec. Spec. Rel. Phenom. **114–116**, 1155 (2001)
22. I.P. Grant, *Relativistic Effects in Atoms and Molecules*, edited by S. Wilson, in Methods in Computational Chemistry (Plenum New York, 1988), Vol. 2, p. 1
23. J.P. Desclaux, Comput. Phys. Commun. **9**, 31 (1975); P. Indelicato, private communications, 2000
24. S. Fritzsche, C.Z. Dong, E. Träbert, Mon. Not. R. Astron. Soc. **318**, 263 (2000)
25. Y.–K. Kim, private communication, 1999
26. S. Fritzsche, C. Froese Fischer, G. Gaigalas, Comp. Phys. Commun. **148**, 103 (2002)
27. C.Z. Dong, S. Fritzsche, B. Fricke, W.–D. Sepp, Mon. Not. R. Astron. Soc. **307**, 809 (1999)
28. S. Fritzsche, I.P. Grant, Phys. Scripta **50**, 473 (1994)
29. S. Fritzsche, B. Fricke, D. Geschke, A. Heitmann, J.E. Sienkiewicz, Astrophys. J. **518**, 994 (1999)
30. S. Fritzsche, I.P. Grant, Phys. Lett. A **186**, 152 (1994)
31. P. Indelicato, Phys. Rev. Lett. **96**, 3323 (1996)
32. A. Derevianko, I.M. Savukov, W.R. Johnson, D.R. Plante, Phys. Rev. A **58**, 4453 (1998)
33. P.O. Löwdin, Phys. Rev. **97**, 1474 (1955)
34. K.T. Cheng, W.R. Johnson, Phys. Rev. A **16**, 263 (1977)
35. A. Hibbert, C. Froese Fischer, M.R. Godefroid, Comp. Phys. Commun. **51**, 285 (1988)
36. J. Olsen, M.R. Godefroid, P. Jösson, P.Å. Malmqvist, C. Froese Fischer, Phys. Rev. E **52**, 4499 (1995)
37. S. Fritzsche, I.P. Grant, Compt. Phys. Commun. **103**, 277 (1997); S. Fritzsche, J. Anton, Comput. Phys. Commun. **124**, 354 (2000)
38. S. Fritzsche, C. Froese Fischer, C.Z. Dong, Comput. Phys. Commun. **124**, 342 (2000)
39. R. Tommasini, F. Lönthal, J.E. Balmer, Phys. Rev. A **59**, 1577 (1999)
40. D. Schneider, Phys. Scripta **59**, 189 (1995)
41. R.E. Marrs, P. Beiersdorfer, S.R. Elliott, D.A. Knapp, Th. Stöhlker, Phys. Scripta **59**, 183 (1995)
42. P.H. Mokler, Th. Stöhlker, Adv. At. Mol. Opt. Phys. **37**, 297 (1996)