

# MCDF and RQDO study of the fine-structure lines of transition array $np^2 \rightarrow np(n+1)s$ in isoelectronic atomic systems

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**Abstract.** Relativistic calculations of electric dipole (E1) allowed transition for a number of ions in the germanium sequence have been performed. Oscillator strengths for fine-structure transitions within the  $4p^2-4p5s$  array have been calculated with both the Multiconfigurational Dirac-Fock (MCDF) approach and the Relativistic Quantum Defect Orbital (RQDO) method. The results are analysed on the grounds of the theoretical data available in the literature. Also, a comparative analysis with the homologous silicon sequence is made. The spectra of systems such as Mo XI are important in the context of plasma physics and thermonuclear fusion measurements.

**Key words.** atomic data – line: identification

## 1. Introduction

The detection of heavy trace elements with nuclear charge numbers  $Z \geq 30$  in the planetary nebula (PN) NGC 7027 (Péquignot & Baluteau 1994) has opened up interesting scientific possibilities in astrophysics. Ge I has been observed in the spectra of Ap and Bp stars (Adelman et al. 1979) and in the solar photosphere (Moore et al. 1966), and the determination of the chemical composition of the stars depends in a sensitive way on the availability of accurate transition probabilities. The study of elemental abundances of heavy elements ( $Z \geq 30$ ) in the interstellar medium allows the exploration of the possible effects of local chemical enrichment and mixing in the interstellar gas and also the nature of the condensation of elements from the gas phase on dust (Savage 1993; Cardelli 1994; Morton 1996). These heavy elements have derived from nuclear processes (slow and rapid neutron captures on to light elements generated by different stellar progenitors) that differ from those producing Zn and the lighter elements (element burning occurring at high temperature, Cameron 1982).

Most atoms and ions in the interstellar medium are observed in their ground energy states because of their low collisional excitation rates, and their resonance lines appear generally in the UV region. The high-resolution gratings of the Goddard High Resolution Spectrograph aboard the Hubble Space Telescope now allow the detection of very weak absorption lines. As a consequence, it becomes possible to investigate absorption lines of some heavy elements, the cosmic abundances of which are rather low (several times smaller than that of hydrogen by number) (Biémont et al. 1998).

Experimentally, the spectra of some Ge-like ions have been analysed. Several transition arrays have been studied for the ions Y VIII – Mo XI (Rahimullah et al. 1976, 1978; Chaghtai et al. 1980; Ateqad et al. 1984) on the basis of spectrograms obtained at Lund University. The  $4p-5s$  transition of Ru XIII, Rh XIV and Pd XV has been observed in laser-produced plasmas by O’Sullivan et al. (1988). Emission spectra of Rb VI (O’Sullivan & Maher 1989) and Sr VII (O’Sullivan 1989) produced by the same technique have been photographed in the 40–500 and 250–500 Å regions, respectively, leading to the identification of a number of transitions.

However, in view of the paucity of experimental data on fine-structure splitting of highly ionized atoms, some theoretical effort has been devoted to prediction of ions with high nuclear charge  $Z$  in order to identify such lines in plasmas. A number of calculations have been done on the ions isoelectronic with Ge, most of them corresponding to allowed transitions. For forbidden transitions, theoretical E2 and M1 transition probabilities along the germanium sequence up to Ag XVI have been published by Biémont & Hansen (1986) and Biémont et al. (1990). However, transition probability data for the highly-ionized germanium-like ions are very scarce. This lack of data, coupled with the consistent set of experimental levels that is now available for the ions Sr VI – Mo XI (Litzén & Reader 1989), justifies new calculations.

For instance, to our knowledge, data on  $4p \rightarrow 5s$  transition probabilities for the whole sequence have not been reported. We have thus considered that there is room for new calculations for the fine structure lines of the above transition in the germanium sequence.

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Along the last decade, we have applied the Relativistic Quantum Defect Orbital (RQDO) method (Martín & Karwowski 1991; Karwowski & Martín 1991; Martín et al. 2000a) to the calculation of oscillator strengths of several isoelectronic sequences (see, e.g. Martín et al. 1991, 1993, 2000b; Charro & Martín 1998; Charro et al. 1997, 2000). The RQDO formalism is a simple but reliable analytical method based on a model Hamiltonian. It has the great advantage that the computational effort does not increase as the atomic system dealt with becomes heavier. The convenience of employing exactly solvable model potentials for calculating atomic transition probabilities manifests itself not only from a practical point of view but also because of the involved physical implications, when they are capable of achieving a good balance between computational effort and accuracy of results. Additionally, and as an independent calculation, we have also applied the multiconfiguration Dirac-Fock (MCDF) formalism, as implemented in the GRASP code (Dyall et al. 1989), to the study of some isoelectronic sequences (Charro et al. 1996, 1997; Charro & Martín 1998).

In the present work, electric dipole (E1) oscillator strengths for several lines within the 4p→5s transition array in the germanium sequence are reported. RQDO and MCDF calculations have been performed on a number of Ge-like ions ranging from Rb VI ( $Z = 37$ ) to Ba XXV ( $Z = 56$ ). Given that some of these ions are heavy and in a high degree of ionization, we expect that the relativistic contributions to the wavefunctions and energies of the levels involved in the present transitions may not be negligible. Also, we find the direct calculation of fine-structure line strengths to be interesting from a spectroscopic point of view. It is of clear usefulness in spectral analyses in astrophysics and fusion plasma research. Whenever previously calculated data were available in the literature, a comparative analysis of the present  $f$ -values has been carried out.

## 2. Relativistic Quantum Defect Orbital calculations

The Relativistic Quantum Defect Orbital (RQDO) method has been described in detail in previous papers (Karwowski & Martín 1991; Martín & Karwowski 1991; Martín et al. 2000a). Therefore, we shall only briefly summarise its most fundamental aspects.

The relativistic quantum defect orbitals are determined by solving analytically the quasi-relativistic scalar second-order Dirac-like equation, obtained after decoupling the radial, two-component Dirac equation, through a non-unitary transformation.

$$\left[ -\frac{d^2}{dr^2} + \frac{\Lambda(\Lambda + 1)}{r^2} - \frac{2Z'_{\text{net}}}{r} \right] \psi_k^{\text{RD}} = 2e^{\text{RD}} \psi_k^{\text{RD}}. \quad (1)$$

The relativistic quantum defect orbitals are expressed in terms of Kummer's functions, where the definition of the parameters can be found in the references above.

$$\psi_k(r)^{\text{RD}} = C \exp\left(\frac{-Z'_{\text{net}} r}{\eta^*}\right) \left(\frac{2Z'_{\text{net}} r}{\eta^*}\right)^{\Lambda+1} \times F\left(-(\eta^* - \Lambda - 1), 2\Lambda + 2, \frac{2Z'_{\text{net}} r}{\eta^*}\right) \quad (2)$$

$C$  is the normalization constant,

$$C = \left(\frac{2Z'_{\text{net}}}{\eta^*}\right)^{1/2} \left[\frac{\Gamma(\eta^* + \Lambda + 1)}{2\eta^* \Gamma(\eta^* - \Lambda)}\right]^{1/2} \frac{1}{\Gamma(2\Lambda + 2)}. \quad (3)$$

With  $\eta^* = \eta - \delta'$ , and

$$\Lambda = \eta - n + l - \delta' + c, \quad (4)$$

$$Z'_{\text{net}} = Z_{\text{net}}(1 + \alpha^2 E^x), \quad (5)$$

$$e^{\text{RD}} = -\frac{(Z'_{\text{net}})^2}{2(\eta - \delta')^2} = E^x \frac{(1 + \alpha^2 E^x/2)}{(1 + \alpha^2 E^x)^2}. \quad (6)$$

Here  $n$  and  $l$  are the principal and orbital angular momentum quantum numbers; and  $\eta$  is the relativistic principal quantum number, related with  $n$  as follows

$$\eta = n - |k| + |s| \quad (7)$$

with

$$s = k(1 - \alpha^2 Z^2/k^2)^{1/2} \quad (8)$$

and

$$k = \epsilon(j + 1/2) \quad (9)$$

where  $\epsilon = \pm 1$ .

$\delta'$  is the relativistic quantum defect,  $c$  is an integer chosen to ensure the normalization of the wavefunction and its correct nodal structure;  $Z'_{\text{net}}$  is the scaled nuclear charge acting on the valence electrons at large radial distances;  $E^x$  is the experimentally measured energy, and  $\alpha$  is the fine structure constant. Atomic units are used throughout.

Since the effective Hamiltonian in Eq. (1) includes a screening term, the quantum defect orbitals are approximately valid in the core region of space. Core polarization effects are implicitly included in the calculations as they are accounted for in the  $\Lambda$  parameter of the model Hamiltonian, as it contains the experimentally determined quantum defect. In some of our previous papers (see e.g., Martín et al. 1989) we have, additionally, introduced a core-polarization correction term in the transition operator. However, it is our experience that moderately – to highly-ionized atoms are rather insensitive to the explicit introduction of a core-polarization correction in the transition moment. This feature is to be expected on the grounds of an increasingly compact core. Therefore, in the present calculations, the standard form of the electric dipole transition operator has been employed. On the other hand, given the one-electron nature of the RQDO formalism, it can be expected to perform better in highly excited states, where the active electron interacts less with the core and other valence electrons, than in low-lying energy states. The relativistic quantum defect orbitals lead to closed-form analytical expressions for the transition integrals. This allows us to calculate transition probabilities and oscillator strengths by simple algebra and with computational efficiency.

The electric dipole oscillator strength for a transition between two states within LSJ-coupling, is given in terms of the radial matrix element by the equation

$$f = \frac{2}{3} \frac{I_m}{2J + 1} \Delta E(R_{\text{line}})^2 (R_{\text{mult}})^2 (-1)^{l-l_m} \times | \langle R_{nlj} | Q(r) | R_{n'l'j'} \rangle |^2 \quad (10)$$

**Table 1.** Experimental energy levels in  $\text{cm}^{-1}$  from different experimental sources.

Level	Rb VI <sup>a</sup>	Sr VII <sup>b</sup>	Y VIII <sup>c</sup>	Zr IX <sup>c</sup>	Nb X <sup>c</sup>	Mo XI <sup>c</sup>
4p <sup>2</sup> <sup>3</sup> P <sub>1</sub>	5120.	6820.	8905.	11365.	14287.	17590.
4p <sup>2</sup> <sup>3</sup> P <sub>2</sub>	9890.	12610.	15565.	18976.	22820.	27136.
4p5s (1/2, 1/2) <sub>0</sub>	303480.	373400.	448870.	529471.	615619.	707195.
4p5s (1/2, 1/2) <sub>1</sub>	304640.	374670.	450242.	531133.	617447.	709073.
4p5s (3/2, 1/2) <sub>2</sub>	313630.	386270.	464847.	549098.	639199.	735189.

<sup>a</sup> O'Sullivan (1989).

<sup>b</sup> O'Sullivan & Maher (1989).

<sup>c</sup> Rahimullah et al. (1978).

where  $l_m$  is the greatest of the orbital angular-momentum quantum numbers of the states involved in the transition,  $(2J + 1)$  is the degeneracy of initial level,  $\Delta E$  is the transition energy in Hartrees,  $R_{\text{line}}$  is a line factor,  $R_{\text{mult}}$  is a multiplet factor,  $\langle R_{nlj} | Q^{(2)} | R_{n'l'j'} \rangle$  is the radial transition integral, and  $Q(r)$  is the standard dipole-length transition operator.

Thus, we define a line factor  $R_{\text{line}}$  by

$$R_{\text{line}}(SLJ, S'L'J') = (2J + 1)^{1/2} (2J' + 1)^{1/2} \times W(SJL'1, LJ') \quad (11)$$

where  $W(SJL'1, LJ')$  are the Racah coefficients which can be described in terms of  $6j$ -symbols

$$W(SJL'1, LJ') = (-1)^{S+J+L'+2} \begin{Bmatrix} S & J & L \\ 1 & L' & J' \end{Bmatrix} \quad (12)$$

and  $R_{\text{mult}}$  may be expressed as follows:

$$R_{\text{mult}}(\alpha L, \alpha' L') = (2L + 1)^{1/2} (2L' + 1)^{1/2} \times W(L_c L L' 1, LL') \quad (13)$$

where  $L_c$  refers to the orbital angular momentum of the atomic core, and the last symbol in Eq. (13) is,

$$W(L_c L L' 1, LL') = (-1)^{L_c+L+L'+2} \begin{Bmatrix} L_c & L & L \\ 1 & L' & L' \end{Bmatrix}. \quad (14)$$

### 3. Multiconfiguration Dirac-Fock calculations

A thorough description of the MCDF method (Grant 1988), as implemented in the GRASP code, can be found in the literature (Dyall et al. 1989). The magnetic and retardation terms to the electron-electron interaction; i.e., the Breit terms, are treated perturbatively by diagonalizing the Dirac-Coulomb-Breit Hamiltonian matrix in the final stage, using the self-consistent orbitals from the first step. To include an estimate of the main radiative corrections to the atomic states, electron self-energies are approximated by scaling hydrogenic results to an effective nuclear charge  $Z_{\text{eff}}$  which is seen by the electrons. The QED corrections to the diagonal elements were added and the vacuum polarization contribution is also included.

The extended average level (EAL) mode (Dyall et al. 1989) has been used in the present calculations. This constructs orbitals from an average energy functional where the fine-structure levels are given the weight  $(2J+1)$ .

The configurations we have included are the following,

4s<sup>2</sup> 4p<sup>2</sup> and 4p<sup>4</sup> to describe the ground configuration.

4s<sup>1</sup> 4p<sup>3</sup> + 4s<sup>2</sup> 4p 5s + 4s<sup>2</sup> 4p 4d to describe the excited configurations.

The choice of these configurations has been made on the grounds of the comments by other authors who have performed similar calculations and by observing that this configuration mixing leads to a good accord between dipole-length (Babushkin gauge) and dipole velocity (Coulomb gauge) MCDF oscillator strengths for most of the transitions studied. To predict the position of the lines, O'Sullivan et al. (1988) performed their calculations using the 4s<sup>2</sup> 4p 5s, 4s<sup>2</sup> 4p 4d and 4s<sup>1</sup> 4p<sup>3</sup> configurations to describe the upper state. Bieroń et al. (1991) studied the  $np^2$ - $np(n+1)s$  transitions in different neutral elements and ions, such as Ge I and As II. These authors report that the  $np^4$  configuration admixed with  $ns^2 np^2$ , and  $ns^1 np^3$  admixed with  $ns^2 np(n+1)s$ . For the ground 4s<sup>2</sup> 4p<sup>2</sup> configuration, Flambaum & Sushkow (1978) and later Biémont & Hansen (1986) found that the highly excited  $np^4$  configuration gives the largest interaction. Similarly, the excited  $ns^2 np(n+1)s$  configuration interacts strongly with states of  $ns^1 np^3$  configuration (Dembczynski & Rebel 1984).

## 4. Discussion of the results

### 4.1. Energy data

In the RQDO context, energy level data are required in order to obtain the quantum defects. For the ions ranging from Rb VI to Mo XI, we have employed the experimental data provided by different authors. The observed energy values by O'Sullivan (1989) for Rb VI and O'Sullivan & Maher (1989) for Sr VII derive from spectra of laser-produced plasmas, where the position of the lines was identified with the help of MCDF calculations, which were also employed to determine  $f$ -values. These authors (O'Sullivan 1989; O'Sullivan & Maher 1989) report a fair agreement between the calculated and observed energies. For the ions Y VIII to Mo XI the experimental energies by Rahimullah et al. (1978) have been employed. Earlier energy data measured by Rahimullah et al. (1976) for these ions are in good agreement with those of Litzén & Reader (1989), reported later. The energies of the levels that we have used in the RQDO calculations are collected in Table 1.

**Table 2.** Fine-structure 4p–5s oscillator strengths for some Ge-like ions.

$J - J'$	Method	0–1	1–0	1–1	1–2	2–1	2–2
Rb VI	<i>RQDO</i> <sup>a</sup>	0.2069	0.0765	0.0554	0.0682	0.0590	0.1322
	<i>MCDF</i> <sup>b</sup>	0.1875	0.0666	0.0441	0.0760	0.0613	0.1352
	<i>OTHER</i>	0.206 <sup>c</sup>	0.078 <sup>c</sup>	0.049 <sup>c</sup>	0.0887 <sup>c</sup>	0.073 <sup>c</sup>	0.153 <sup>c</sup>
Sr VII	<i>RQDO</i> <sup>a</sup>	0.1892	0.0663	0.0490	0.0704	0.0505	0.1310
	<i>MCDF</i> <sup>b</sup>	0.1891	0.0689	0.0445	0.0795	0.0710	0.1374
	<i>OTHER</i>	0.204 <sup>d</sup>	0.0775 <sup>d</sup>	0.0475 <sup>d</sup>	0.0879 <sup>d</sup>	0.0766 <sup>d</sup>	0.147 <sup>d</sup>
Y VIII	<i>RQDO</i> <sup>a</sup>	0.1872	0.0658	0.0487	0.0693	0.0501	0.1290
	<i>MCDF</i> <sup>b</sup>	0.1905	0.0736	0.0447	0.0808	0.0765	0.1344
Zr IX	<i>RQDO</i> <sup>a</sup>	0.1863	0.0658	0.0486	0.0688	0.0501	0.1279
	<i>MCDF</i> <sup>b</sup>	0.1906	0.0746	0.0444	0.0811	0.0810	0.1293
Nb X	<i>RQDO</i> <sup>a</sup>	0.1860	0.0659	0.0488	0.0685	0.0502	0.1273
	<i>MCDF</i> <sup>b</sup>	0.1898	0.0751	0.0440	0.0810	0.0848	0.1230
Mo XI	<i>RQDO</i> <sup>a</sup>	0.1810	0.0644	0.0477	0.0661	0.0491	0.1229
	<i>MCDF</i> <sup>b</sup>	0.1887	0.0753	0.0436	0.0806	0.0881	0.1164

<sup>a</sup> Relativistic Quantum Defect Orbital Method, present work.

<sup>b</sup> Multiconfiguration Dirac-Fock, this work.

<sup>c</sup> O'Sullivan (1989).

<sup>d</sup> O'Sullivan & Maher (1989).

Other input data also needed in the RQDO calculations are the ionization energies of the atomic systems. The values adopted for Rb VI to Mo XI are those supplied by Fraga et al. (1976). For the remaining ions, no RQDO calculations were performed given the lack of ionization energies in the literature. For these we only supply MCDF results.

#### 4.2. Fine-structure oscillator strengths for the 4p–5s transition array

In Tables 2 and 3, we display the  $f$ -values obtained in the present work together with the theoretical values reported by other authors. Inspection of Table 2 shows that the magnitudes of our RQDO and MCDF oscillator strengths are, in general, in fairly good agreement, and compare well, in most cases, with the  $f$ -values calculated by O'Sullivan (1989) for Rb VI and O'Sullivan & Maher (1989) for Sr VII. These data have been obtained by combining experimental and theoretical (MCDF) results for the identification of the lines in the Rb VI and Sr VII spectra. It should be borne in mind that some of the levels involved in the transition can be subject to perturbations by other levels. These perturbations are explicitly accounted for in the MCDF calculations, whilst in the RQDO procedure, the effect of perturbations is only implicitly included through the quantum defects extracted from experimental energies. In Table 3, the MCDF results are collected together with data for Ru XIII, Rh XIV and Pd XV reported by O'Sullivan et al. (1988). These authors analysed the different spectra in the way described above. In this table, for the  $J = 0 \rightarrow J' = 1$  absorption line, a good agreement between our

calculations and the comparative value is apparent, but some sizable differences can be observed for other lines in the transition array. A source of discrepancy between the MCDF  $f$ -values and those by O'Sullivan et al. (1988) are very likely the different configurations included in the two calculations. The extra configuration ( $4p^4$ ) we have added, as compared with those included by O'Sullivan et al. (1988), may have a lot to do with the discrepancies.

A comparative analysis with the MCDF oscillator strengths recently obtained by us (Charro et al. 1997) for the silicon isoelectronic sequence, which is homologous to the presently studied Ge sequence, may be taken as a good basis for a justification of the choice of the configurations now included in the MCDF procedure. In our calculations of the fine-structure transitions within the  $3p^2 \rightarrow 3p4s$  array in the silicon sequence, which is homologous to the  $4p^2 \rightarrow 4p5s$  array in the Ge isoelectronic sequence, the inclusion of the  $3p^4$  configuration was found to yield the best ground state energy (Charro et al. 1997).

Table 4 displays the  $f$ -values for the 4p–5s multiplet transition deduced from the sum rules (Cowan 1981), also applied in previous calculations (Charro et al. 1996). Table 4 reveals a good compliance with the sum rule by all the three sets of oscillator strengths for Rb VI and Sr VII, as well as close similarities in the magnitude of our MCDF and RQDO calculations. However, for the remaining three ions, only our calculations appear to satisfy the sum rule. This might be due to a change in the coupling scheme from sr VII to Ru XIII, not well accounted for in the data reported by O'Sullivan et al. (1988). Our MCDF calculations have been performed in such a way that the coupling scheme is automatically changed by the GRASP program when required.

**Table 3.** Fine-structure 4p–5s oscillator strengths for some Ge-like ions, the first entry: MCDF<sup>a</sup>, second entry: O’Sullivan et al.<sup>2</sup>

ION	Method	0–1	1–0	1–1	1–2	2–1	2–2
Ru XIII	MCDF <sup>a</sup>	0.1858	0.0755	0.0426	0.0793	0.0934	0.1035
	OTHER <sup>b</sup>	0.187	0.025	0.014	0.026	0.019	0.0202
Rh XIV	MCDF <sup>a</sup>	0.1843	0.0755	0.0422	0.0786	0.0956	0.0976
	OTHER <sup>b</sup>	0.186	0.025	0.014	0.026	0.019	0.019
Pd XV	MCDF <sup>a</sup>	0.1826	0.0755	0.0418	0.0779	0.0975	0.0921
	OTHER <sup>b</sup>	0.185	0.025	0.014	0.026	0.019	0.018
Ag XVI	MCDF <sup>a</sup>	0.1810	0.0755	0.0415	0.0771	0.0991	0.0872
Cd XVII	MCDF <sup>a</sup>	0.1794	0.0755	0.0412	0.0764	0.1005	0.0828
In XVIII	MCDF <sup>a</sup>	0.1778	0.0756	0.0410	0.0757	0.1018	0.0788
Sn XIX	MCDF <sup>a</sup>	0.1763	0.0756	0.0408	0.0749	0.1030	0.0752
Sb XX	MCDF <sup>a</sup>	0.1747	0.0758	0.0406	0.0743	0.1041	0.0720
Te XXI	MCDF <sup>a</sup>	0.1732	0.0759	0.0405	0.0736	0.1052	0.0691
I XXII	MCDF <sup>a</sup>	0.1718	0.0761	0.0404	0.0729	0.1052	0.0666
Xe XXIII	MCDF <sup>a</sup>	0.1703	0.0763	0.0403	0.0723	0.1071	0.0642
Cs XXIV	MCDF <sup>a</sup>	0.1689	0.0766	0.0403	0.0717	0.1081	0.0621
Ba XXV	MCDF <sup>a</sup>	0.1676	0.0768	0.0403	0.07107	0.1090	0.0602

<sup>a</sup> Multiconfiguration Dirac-Fock, this work.

<sup>b</sup> O’Sullivan et al. (1988).

### 4.3. Regularities in homologous series

Regularities in individual oscillator strengths along an isoelectronic sequence as functions of the nuclear charge are predicted from conventional perturbation theory (Cohen & Dalgarno 1966; Dalgarno & Parkinson 1967), and their usefulness in analysing the  $f$ -values has been repeatedly stressed (see, e.g., Martin & Wiese 1996 and references therein).

The oscillator strengths for strong analogous ( $nl \rightarrow n'l'$ ) transitions of homologous atoms are expected to be similar on account of the similar outer electron structure of such elements. However, one has to consider that as the elements within a chemical family become heavier, the outer atomic structure may become modified due to the presence of unfilled electron shells. In this sense, germanium-like ions, with a completely filled M shell, have a similar outer atomic structure to that of the Si-like ions, but these have the 3d shell unfilled. Generally, the systematic behaviour of homologous atoms is not expected to be as closely adhered to as for the case of a given transition along an isoelectronic sequence, where the electron configuration remains the same and only a scaling of the nuclear charge occurs, but it is observed in some cases. As an illustration, Fig. 1 displays the behaviour of the fine-structure lines of

the  $np^2 \rightarrow np(n+1)s$  transition arrays of the Si and Ge isoelectronic sequences, where  $n = 3$  and 4, respectively, against  $\xi$ .  $\xi$  is defined as the effective nuclear charge on the active electron ( $\xi = Z - N$ ), where  $Z$  is the nuclear charge and  $N$  is the number of core electrons. In this way, following the spectroscopic notation, for a neutral atom we have  $\xi = 1$ .

## 5. Conclusions

The RQDO procedure has once more proved to be a useful tool for estimating transition probabilities. In the particular case of the Ge-like ions, a general, satisfying, agreement is found between the RQDO results and those obtained with rather more elaborate procedures, such as MCDF. Nearly parallel  $f$  versus  $\xi$  curves have been obtained for some representative analogous fine-structure lines along the homologous Ge and the previously studied (Charro et al. 1997) Si isoelectronic sequences. This feature may be interpreted as proof of the internal consistency of our calculations.

We are confident that the  $f$ -values we supply for some heavy ions isoelectronic with germanium may be potentially useful in astrophysics and fusion plasma research.

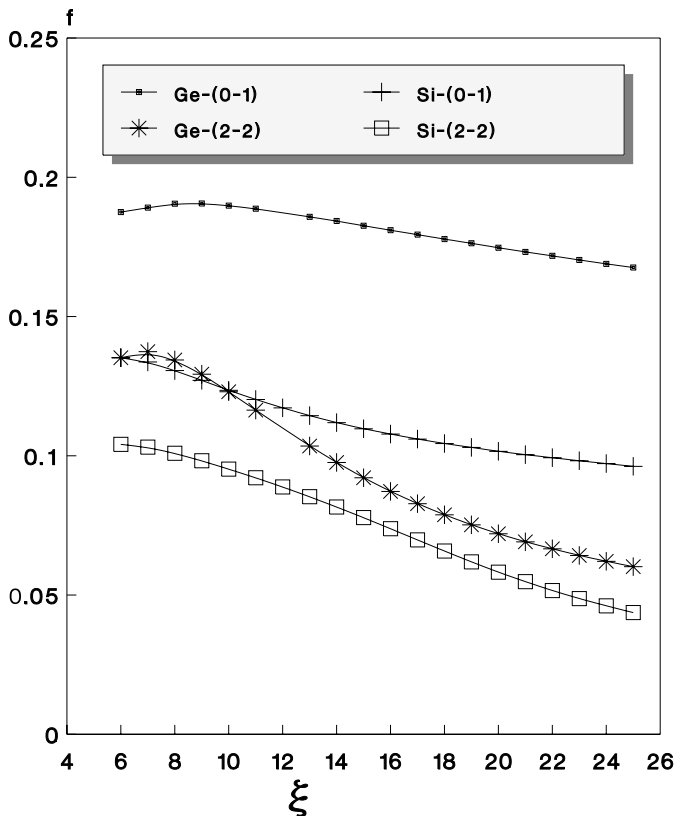
**Table 4.** Comparison of oscillator strengths for the multiplet transition 4p–5s following the sum rule.

ION	$J - J'$	<i>OTHER</i>	<i>MCDF</i> <sup>d</sup>	<i>RQDO</i> <sup>e</sup>
Rb VI	0 – 1	0.206 <sup>a</sup>	0.1875	0.2069
	1 – 0, 1, 2	0.2157 <sup>a</sup>	0.1867	0.2001
	2 – 1, 2	0.226 <sup>a</sup>	0.1965	0.1912
Sr VII	0 – 1	0.204 <sup>b</sup>	0.1891	0.1892
	1 – 0, 1, 2	0.2129 <sup>b</sup>	0.1929	0.1857
	2 – 1, 2	0.2236 <sup>b</sup>	0.2084	0.1815
Ru XIII	0 – 1	0.187 <sup>c</sup>	0.1858	-
	1 – 0, 1, 2	0.065 <sup>c</sup>	0.1974	-
	2 – 1, 2	0.0392 <sup>c</sup>	0.1969	-
Rh XIV	0 – 1	0.186 <sup>c</sup>	0.1843	-
	1 – 0, 1, 2	0.065 <sup>c</sup>	0.1963	-
	2 – 1, 2	0.038 <sup>c</sup>	0.1932	-
Pd XV	0 – 1	0.185 <sup>c</sup>	0.1826	-
	1 – 0, 1, 2	0.065 <sup>c</sup>	0.1952	-
	2 – 1, 2	0.037 <sup>c</sup>	0.1896	-

<sup>a</sup> O'Sullivan (1989).<sup>b</sup> O'Sullivan & Maher (1989).<sup>c</sup> O'Sullivan et al. (1988).<sup>d, e</sup> Present work.**Table 5.** Fine-structure 4p–5s RQDO oscillator strengths for Ge-like ions (*a*) and Si-like ions (*b*).

ION	0–1	1–0	1–1	1–2	2–1	2–2
Rb VI	0.2069 <sup>a</sup>	0.0765 <sup>a</sup>	0.0554 <sup>a</sup>	0.0682 <sup>a</sup>	0.0590 <sup>a</sup>	0.1322 <sup>a</sup>
K VI	0.1724 <sup>b</sup>	0.0581 <sup>b</sup>	0.0433 <sup>b</sup>	0.07060 <sup>b</sup>	0.0436 <sup>b</sup>	0.1280 <sup>b</sup>
Sr VII	0.1892 <sup>a</sup>	0.0663 <sup>a</sup>	0.0490 <sup>a</sup>	0.0704 <sup>a</sup>	0.0505 <sup>a</sup>	0.1310 <sup>a</sup>
Ca VII	0.1709 <sup>b</sup>	0.0577 <sup>b</sup>	0.0430 <sup>b</sup>	0.0698 <sup>b</sup>	0.0433 <sup>b</sup>	0.1267 <sup>b</sup>
Y VIII	0.1872 <sup>a</sup>	0.0658 <sup>a</sup>	0.0487 <sup>a</sup>	0.0693 <sup>a</sup>	0.0501 <sup>a</sup>	0.1290 <sup>a</sup>
Sc VIII	0.1695 <sup>b</sup>	0.0573 <sup>b</sup>	0.0427 <sup>b</sup>	0.0690 <sup>b</sup>	0.0431 <sup>b</sup>	0.1253 <sup>b</sup>
Zr IX	0.1863 <sup>a</sup>	0.0658 <sup>a</sup>	0.0486 <sup>a</sup>	0.0688 <sup>a</sup>	0.0501 <sup>a</sup>	0.1279 <sup>a</sup>
Ti IX	0.1678 <sup>b</sup>	0.0568 <sup>b</sup>	0.0423 <sup>b</sup>	0.0680 <sup>b</sup>	0.0427 <sup>b</sup>	0.1238 <sup>b</sup>
Nb X	0.1860 <sup>a</sup>	0.0659 <sup>a</sup>	0.0488 <sup>a</sup>	0.0685 <sup>a</sup>	0.0502 <sup>a</sup>	0.1273 <sup>a</sup>
V X	0.1706 <sup>b</sup>	-	0.0430 <sup>b</sup>	0.0690 <sup>b</sup>	0.0435 <sup>b</sup>	0.1257 <sup>b</sup>
Mo XI	0.1810 <sup>a</sup>	0.0644 <sup>a</sup>	0.0477 <sup>a</sup>	0.0661 <sup>a</sup>	0.0491 <sup>a</sup>	0.1229 <sup>a</sup>
Cr XI	0.1697 <sup>b</sup>	0.0576 <sup>b</sup>	0.0429 <sup>b</sup>	0.0685 <sup>b</sup>	0.0434 <sup>b</sup>	0.1248 <sup>b</sup>

<sup>a</sup> Present work.<sup>b</sup> Charro et al. (1997).



**Fig. 1.** Systematic trends for three fine-structure  $np^2 \rightarrow np(n+1)s$  transitions of the Si and Ge sequences ( $n = 3$  and 4, respectively). For both sequences, our MCDF oscillator strengths are plotted versus  $\xi$ , the charge on the atomic core or effective nuclear charge. Several symbols are used for the different lines ( $J - J'$ ).

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## References

- Adelman, S., Bidelman, W. P., & Pyper, D. 1979, *ApJ*, 40, 371
- Ateqad, N., Chaghtai, M. S. Z., & Rahimullah, K. 1984, *J. Phys. B*, 17, 4617
- Biéumont, E., & Hansen, J. E. 1986, *Phys. Scr.*, 33, 117
- Biéumont, E., Himdy, A. El, & Garnir, H. P. 1990, *J. Quant. Spectrosc. Radiat. Transfer*, 43(6), 437
- Biéumont, E., Morton, D. C., & Quinet, P. 1998, *MNRAS*, 297, 713
- Bieroń, J. R., Marcinek, R., & Migdalek, J. 1991, *J. Phys. B*, 24, 31
- Cameron, A. G. W. 1982, *Essays in Nuclear Astrophysics* (Cambridge Univ. Press, Cambridge)
- Cardelli, J. A. 1994, *Sciences*, 265, 209
- Chaghtai, M. S. Z., Khan, Z. A., & Rahimullah, K. 1980, *J. Phys. B*, 13, 2523
- Charro, E., & Martín, I. 1998, *A&AS*, 131, 523
- Charro, E., Martín, I., & Lavín, C. 1996, *J. Quant. Spectrosc. Radiat. Transfer*, 56, 241
- Charro, E., Martín, I., & Lavín, C. 1997, *A&AS*, 124, 397
- Charro, E., Martín, I., & Serna, M. A. 2000, *J. Phys. B*, 33, 1753
- Cowan, R. D. 1981, *The Theory of Atomic Structure and Spectra* (Univ. of California Press)
- Cohen, M., & Dalgarno, A. 1966, *Proc. Roy. Soc. (London)*, A293, 359
- Dalgarno, A., & Parkinson, E. M. 1967, *Proc. Roy. Soc. (London)*, A301, 253
- Dembczynski, J., & Rebel, H. 1984, *Physica*, 125C, 341
- Dyall, K. G., Grant, I. P., Johnson, C. T., Parpia, F. A., & Plummer, E. P. 1989, *Comput. Phys. Commun.*, 55, 425
- Flambaum, V. V., & Sushkov, O. P. 1978, *J. Quant. Spectrosc. Radiat. Transfer*, 20, 569
- Fraga, S., Karwowski, J., & Saxena, K. M. S. 1976, *Handbook of Atomic Data* (Elsevier, New York)
- Grant, I. P. 1988, *Meth. Comp. Chem.* 2, ed. S. Wilson, (Plenum Press, New York), 1
- Karwowski, J., & Martín, I. 1991, *Phys. Rev. A*, 43, 4832
- Litzén, U., & Reader, J. 1989, *Phys. Scr.*, 39, 468
- Martín, I., Barrientos, C., & Gutiez, I. 1989, *Int. J. Quant. Chem.*, 36, 205
- Martín, I., & Karwowski, J. 1991, *J. Phys. B*, 24, 1539
- Martín, I., Karwowski, J., & Bielinska-Waz 2000b, *J. Phys. A*, 33, 823
- Martín, I., Karwowski, J., Diercksen, G. H. F., & Barrientos, C. 1993, *A&AS*, 100, 595
- Martín, I., Karwowski, J., Lavín, C., & Diercksen, G. H. F. 1991, *Phys. Scr.*, 44, 567
- Martín, I., Lavín, C., & Charro, E. 2000a, in *Quant. Syst. Phys. Chem. 2: Advanced Problems and Complex Systems*. ed. J. Maruani et al. (Kluwer Academic Publishers, Dordrecht)
- Martin, W. C., & Wiese, W. L. 1996, in *Atomic, Molecular, and Optical Physics Handbook*, ed. G. W. F. Drake (American Institut of Physics, Woodbury, New York), 135
- Moore, C. E., Minnaert, M. G. J., & Houtgast, J. 1966, *The Solar Spectrum 2935-8770 Å* Nat. Bur. Stand. (U.S.) Monograph 61 (U.S. GPO, Washington, DC)
- Morton, D. C. 1996, in *4th International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas*, ed. W.-U.L. Tchang-Brillet, J.-L. Wyart, & C. Zeippen (Publications de l'Observatoire de Meudon, Paris-Meudon), 156
- O'Sullivan, G. 1989, *J. Phys. B*, 22, 987
- O'Sullivan, G., Costello, J. T., Kane, M., & Carrol, P. K. 1988, *J. Phys. B*, 21, L195
- O'Sullivan, G., & Maher, M. 1989, *J. Phys. B*, 22, 377
- Péquignot, D., & Baluteau, J.-P. 1994, *A&A*, 283, 593
- Rahimullah, K., Chaghtai, M. S. Z., & Khatoon, S. 1976, *Phys. Scr.*, 14, 221
- Rahimullah, K., Chaghtai, M. S. Z., & Khatoon, S. 1978, *Phys. Scr.*, 18, 96
- Savage, B. D. 1993, *Phys. Scr.*, T47, 171