

Oscillator strengths in the silicon sequence: Relativistic Quantum Defect Orbital and Multiconfigurational Dirac-Fock calculations

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Abstract. Oscillator strengths for $3s^2 3p^2 \rightarrow 3s^2 3p^1 3d^1$ and $3s^2 3p^2 \rightarrow 3s^2 3p^1 4s^1$ transitions in the silicon sequence (KVI - XeXLI) have been calculated using the Relativistic Quantum Defect Orbital (RQDO) method, with and without explicit inclusion of core-valence correlation, and the multiconfigurational Dirac-Fock (MCDF) approach. Our f -values, which are of interest in astrophysics and fusion plasma research, are compared with other theoretical results in the cases for which these are available.

Key words: atomic data — atomic processes

1. Introduction

Excitation energies and oscillator strengths in highly stripped ions are needed for estimating the energy loss through impurity ions in fusion plasmas and for diagnostics and modelling of the plasmas. Precision spectroscopy both in astrophysical and in beam-foil measurements also demands accurate theoretical values. Furthermore, the systematic trends in atomic structure with respect to the nuclear charge Z can best be studied along an isoelectronic sequence.

Some of the strong lines appearing in laboratory plasmas or in astrophysical sources belong to the $n = 3 \rightarrow n' = 3$ transition arrays of the silicon sequence. Their role in solar identifications is very important; for example, FeXIII is well represented in the solar spectrum, photographed under quiet solar conditions (Behring et al. 1976) or in solar flares (Dere 1978).

Highly ionized members of the silicon isoelectronic sequence have recently been investigated. A comprehensive study of the spectra of Si-like ions between CuXVI and MoXXIX has been reported by Sugar et al. (1990).

This work has since then been extended to KrXXIII and MoXXIX by Jupén et al. (1991), and to GeXIX, SeXXI, SrXXV, YXXVI and ZrXXVII by Ekberg et al. (1992).

Several investigations of energies and oscillator strengths for Si-like ions have also appeared in the literature. For the neutral atom SiI and the first ions of its sequence there are some experimental and theoretical studies (Ho & Henry 1987; Ryan et al. 1989; Becker et al. 1980; O'Brien & Lawler 1991; Livingston et al. 1981; Mendoza & Zeippen 1988; Nahar & Pradhan 1993). Opacity calculations by Nahar & Pradhan (1993) are the most recent theoretical study of SiI, SiII, ArV and Ca VII. For instance, Biémont (1986a, 1986b), Bromage (1980), and Bromage et al. (1978), have applied the relativistic Hartree-Fock (HXR) code of Cowan (1981) to some ions. Their work is semiempirical in the sense that the Slater integrals were adjusted to optimize the agreement with experimental level energies. Using the multiconfiguration Dirac-Fock (MCDF) program of Desclaux (1975), Huang (1985) has performed fully relativistic ab initio calculations for Si-like ions in the range $Z = 15 - 106$.

Among the standard methods suitable for predicting oscillator strengths for transitions in highly ionized and in heavy atoms, the multiconfiguration Dirac-Fock approach seems to be one of the most reliable ones (Dyall et al. 1989). However, this approach becomes too time-consuming if the number of transitions to be determined is very large. According to Curtis (1987), the spectroscopic classification of the relevant lines exceeds the general capability of ab initio methods, and sometimes requires the application of semiempirical methods. Recently, Laughlin (1992) pointed out, after comparing lifetimes obtained with a numerical Coulomb approximation and a model potential with accurate experimental measurements for some alkali-like systems, that high accuracy may be achieved with relatively simple computational procedures, as long as they are appropriate to the problem.

The structure of Si-like ions is quite interesting from the atomic physics point of view. There are four electrons

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outside the closed $2p^6$ shell and the number of configurations within the $n = 3$ complex is 12. The ground level is $3s^2 3p^2 {}^3P_0$, and there are two low-lying metastable levels, $3s^2 3p^2 {}^1D_2$ and 1S_0 .

In these work we report oscillator strengths for the singlet-singlet transitions: $3s^2 3p^2 {}^1D_2 - 3s^2 3p^1 3d^1 {}^1D_2$, $3s^2 3p^2 {}^1D_2 - 3s^2 3p^1 3d^1 {}^1F_3$, $3s^2 3p^2 {}^1D_2 - 3s^2 3p^1 4s^1 {}^1P_1$, as well as for the fine structure lines of the multiplet $3s^2 3p^2 {}^3P - 3s^2 3p^1 4s^1 {}^3P$ in silicon-like ions ranging from KVI up to XeXLI. Systematic trends are analysed by plotting our f -values versus the reciprocal of the atomic number, Z . The calculations have been done with two different approaches, the semiempirical Relativistic Quantum Defect Orbital (RQDO) method (Simons 1974; Martín & Simons 1976; Lavín et al. 1992; Karwowski & Martín 1991; Martín et al. 1993), where in some cases the importance of the polarization of the core by the active electron has been stressed, and the MCDF formalism using the code by Dyall et al. (1989), in the cases where there is not any other MCDF result reported in the literature.

This is the most complex electronic structure to which the RQDO method has so far been applied. In this respect, our calculations will serve as a test on the capability of such a simple formalism for providing good estimates of oscillator strengths in complex systems. A further incentive for this study has been the lack of experimental data for oscillator strengths in these transitions, as well as the fact that only a calculation has been reported, to our knowledge, for the highly ionized atoms of the sequence (Huang 1985).

2. Computational procedures

2.1. Relativistic quantum defect orbital method

The Quantum Defect Orbital (QDO) (Simons 1974; Martín & Simons 1976; Lavín et al. 1992) formalism and its relativistic (RQDO) (Karwowski & Martín 1991; Martín et al. 1993) version have been described in detail. We shall, thus, only mention here some aspects of the theory that are relevant to the present calculations.

The relativistic quantum defect orbitals are determined by solving analytically a quasirelativistic second-order Dirac-like equation with a model Hamiltonian that contains the quantum defect (Karwowski & Martín 1991). This model Hamiltonian allows for an effective variation of the screening effects with the radial distance and as a consequence, the radial solutions behave at least approximately correctly in the core region of space, and display a correct behaviour at large radial distances. These can be expected to be, in most cases, the most relevant regions that contribute to the transition integral. 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 little computational effort. The LS coupling scheme has been adopted in all the studied transitions.

One aspect of the computational procedure which has to be investigated is how to correct the transition operator for the neglect of explicit core-valence correlation in the quantum defect orbitals. It is well known that core-valence correlation significantly contributes to certain transition matrix elements. Laughlin (1989) has pointed out that when matrix elements are calculated with wavefunctions obtained from a valence-electron equation, core-polarization corrections introduced in the transition operator are especially adequate. Different forms for these corrections can be found in the literature. As in some of our previous computations (Lavín et al. 1993) we have adopted (Bielínska-Waz 1992)

$$Q(r) = r \left[1 - \frac{\alpha}{r^3} [1 - \exp(-r/r_c)]^3 \right]$$

where α is the core-polarizability and r_c is a cutoff radius. This expression offers the great advantage, unlike the one formerly proposed by Caves & Dalgano (1972), of retaining total analyticity in the RQDO transition integrals.

In the Relativistic Quantum Defect Orbital (RQDO) method energy level data are required in order to obtain the quantum defects. We have taken the available energy data from the most recent critical compilation (Kelly 1987). For CuXVI to Kr XXIII we have used the energy values by Sugar et al. (1990) and for RbXXIV to MoXXIX those reported by different authors (Sugar et al. 1990; Jupén et al. 1991; Ekberg et al. 1992).

Concerning the accuracy of these energy data, the energy levels reported in the critical compilation (Kelly 1987) are only the lines that have been observed (not calculated). The rest of the experimental sources (Sugar et al. 1990; Jupén et al. 1991; Ekberg et al. 1992) are quite more explicit as to the procedures followed in obtaining their data. Sugar et al. (1990) employed tokamak-generated plasmas for Cu to Mo ions, and laser-produced plasmas for Cu to As ions. Jupén et al. (1991) used the JET tokamak for their experimental measurements. And Ekberg et al. (1992) produced linear plasmas in a line-focused laser beam. In the three cases the wavelengths for the different transitions observed were combined with calculated ones (through relativistic methods). Then, the difference between these quantities was plotted against the atomic number for the isoelectronic sequence, smooth curves being obtained in all cases. This fact allowed the authors to make interpolations for non-observed ions. The wavelengths were then used to derive energy levels. Sugar et al. (1990) claim the uncertainty of observed wavelengths to be $\pm 0.005 \text{ \AA}$ and that of their assignments to be of $\pm 0.020 \text{ \AA}$. Jupén et al. (1991) conclude that their results confirm Sugar et al. (1990)'s findings and claim the tokamaks to be highly competitive light sources for accurate spectroscopy of highly charged ions. Finally, Ekberg

et al. (1992) remark that from their isoelectronic comparisons smooth energies for ions not observed by them have also been obtained, and all their results are in agreement with those reported by Sugar et al. (1990).

The above analyses made us confident in the correctness of the aforementioned energy data and decided to employ them in our calculations. Still there were some gaps in the energy data as regards some of the presently studied ions. These gaps have been filled by our own energy values calculated with the MCDF code as developed by Dyall et al. (1989).

The ionization energies (I.P.) are also needed for our calculations. The values corresponding to the ions with Z -values up to 36 have been taken from Kelly (1987). However, for obtaining the ionization energies from RbXXIV upwards, we have used a Z -dependent expression for extrapolating the I.P. which has been obtained by applying a standard least-squares fitting routine for the data comprised between $Z = 24$ (CrXI) and $Z = 36$ (KrXXIII). The quality of the fit can be evaluated through its correlation factor ($r = 0.9996465$).

Oscillator strengths have been computed both with and without explicit introduction of core polarization effects in the dipole transition operator. For the former, we have taken core polarizabilities from Fraga et al. (1976). Since there is no analytical way of obtaining the cutoff radius r_c , we have chosen a value equal to the core mean radius, calculated in accord with an expression given by Chichkov & Shevelko (1981). In the RQDO calculations where the standard dipole-length transition operator is employed $Q(r) = r$, core-valence polarization is always accounted for implicitly through the semiempirical parameter of the model Hamiltonian.

2.2. Multiconfiguration Dirac-Fock method

The MCDF method, as implemented in the code we have employed (Dyall et al. 1989), is a generalization of the Dirac-Fock formalism, using a multiconfigurational trial function in the variation of the total energy. Within this model, an atomic state function is represented as a linear combination of configuration state functions built from antisymmetrized products of standard Dirac orbitals. These orbitals are eigen-functions of the one-electron total angular momentum operator rather than of the spin and orbital momentum operators independently (as it is the case in the non-relativistic multiconfigurational Hatree-Fock method). For details of the atomic MCDF model we refer to the review by Grant (1988).

The extended average level (EAL) mode (Dyall et al. 1989) has been used in the present calculations. We have chosen the results evaluated with the Babushkin gauge, given that they seem to be the most adequate ones in this context, given that in the relativistic limit, the Babushkin gauge corresponds to the length form of the matrix elements.

In order to achieve accurate results with this method, the most important configurations have been included. For the ground configuration $3s^2 3p^2$, several authors (Flambaum & Sushkov 1978; Biémont & Hansen 1986) found that the highly excited $3p^4$ configuration gives the largest interaction. Similarly, the excited $3s^2 3p^1 4s^1$ configuration interacts strongly with states of the $3s^1 3p^3$ configuration (Dembczynski & Rebel 1984). The important perturbation that appears between $3s^1 3p^3$ and $3s^2 3p^1 3d^1$ is particularly important for the 1D_2 term, as Biémont (1986a) noticed. Consequently, these configurations have been included in our MCDF calculations for the ground and excited states. Computations which add the far-off configurations in which one electron belongs to highly excited orbitals have not been performed, given that the effects of these interactions may be considered to be negligible in calculating both energy levels and oscillator strengths.

3. Results

In Tables 1, 2 and 3, we display the f -values obtained in the present work together with theoretical values reported by other authors, given that no experimental measurements have been found in the literature. In the figures we show the systematic trends that some of the studied oscillator strengths present for individual transitions along the isoelectronic sequence when they are plotted versus the inverse of Z .

For $3s^2 3p^2 \ ^3P - 3s^2 3p^1 4s^1 \ ^3P$ transition we have performed both RQDO and MCDF calculations. Inspection of Table 1 shows that our oscillator strengths compare generally well with the f -values calculated by Biémont (1986a, 1986b), who combined the self-consistent field (HXR) method of Cowan (1981), which explicitly accounts for configuration interaction and some relativistic effects for obtaining the wave functions with a semiempirical fitting procedure for obtaining the energy eigenvalues. Biémont reports f -values (1986a) for the first few ions of the sequence only. Our RQDO f -values take explicitly into account core-polarization effects. It should be born in mind that some of the levels involved in the transition can be subjected to perturbations by other levels, as pointed out by Biémont (1986a). These perturbations are explicitly accounted for in the MCDF calculations. In the RQDO procedure, the effect of perturbations is only implicitly included through the quantum defects extracted from experimental energies. Overall, the RQDO f -values agree reasonably well with the MCDF results and these by Biémont (1986a, 1986b), both expected to be correct. A source of discrepancy between the RQDO and HXR (Biémont 1986a) f -values is, quite possibly, the use of different energy data. Both the RQDO and MCDF results, as well as the HXR f -values, comply with the general feature which characterises an LS coupling scheme (Cowan 1981), in all ions comprised in Table 1, of reflecting that the strongest

Table 1. Oscillator strengths for the lines of the multiplet $3s^2 3p^2 \ ^3P - 3s^2 3p^1 4s^1 \ ^3P$. The first entry (a) corresponds to the values calculated by us with the MCDF code written by Dyllal et al. (1989); the second entry (b) corresponds to our RQDO results including polarization effects, and the third entry (c) corresponds to the values obtained by Biémont (1986a) with the HXR method, as described in the text

Z	ION	M	$^3P_0 - ^3P_1$	$^3P_1 - ^3P_0$	$^3P_1 - ^3P_1$	$^3P_1 - ^3P_2$	$^3P_2 - ^3P_1$	$^3P_2 - ^3P_2$
19	KVI	a.	0.1352	0.0468	0.0337	0.0569	0.0360	0.1041
		b.	0.1724	0.0581	0.0433	0.0706	0.0436	0.1280
		c.	0.1413	0.0482	0.0349	0.0621	0.0372	0.1099
20	CaVII	a.	0.1337	0.0467	0.0332	0.0565	0.0362	0.1031
		b.	0.1709	0.0577	0.0430	0.0698	0.0433	0.1267
		c.	0.1380	0.0482	0.0333	0.0607	0.0364	0.1074
21	ScVIII	a.	0.1306	0.0460	0.0323	0.0554	0.0361	0.1009
		b.	0.1695	0.0573	0.0427	0.0690	0.0431	0.1253
		c.	0.1349	0.0460	0.0318	0.0593	0.0364	0.1026
22	TiIX	a.	0.1271	0.0451	0.0312	0.0541	0.0361	0.0982
		b.	0.1678	0.0568	0.0423	0.0680	0.0427	0.1238
		c.	0.1288	0.0450	0.0304	0.0566	0.0364	0.0980
23	VX	a.	0.1235	0.0443	0.0300	0.0528	0.0362	0.0952
		b.	0.1706	-	0.0430	0.0690	0.0435	0.1257
24	CrXI	a.	0.1202	0.0434	0.0289	0.0516	0.0375	0.0921
		b.	0.1697	0.0576	0.0429	0.0685	0.0434	0.1248
25	MnXII	a.	0.1172	0.0427	0.0279	0.0504	0.0372	0.0888
		b.	0.1683	-	0.0426	0.0677	0.0431	0.1234
26	FeXIII	a.	0.1144	0.0420	0.0269	0.0493	0.0380	0.0853
		b.	-	0.0581	-	0.0664	-	0.1212
27	CoXIV	a.	0.1119	0.0414	0.0260	0.0483	0.0390	0.0816
		b.	0.1512	-	0.0384	0.0660	0.0390	0.1207
28	NiXV	a.	0.1097	0.0408	0.0252	0.0473	0.0402	0.0778
		b.	-	-	-	0.0642	-	0.1196
29	CuXVI	a.	0.1078	0.0403	0.0245	0.0465	0.0414	0.0738
		b.	0.1607	0.0551	0.0410	0.0636	0.0415	0.1162
30	ZnXVII	a.	0.1060	0.0399	0.0239	0.0456	0.0427	0.0698
		b.	0.1586	0.0546	0.0406	0.0620	0.0412	0.1135
31	GaXVIII	a.	0.1044	0.0395	0.0233	0.0449	0.0439	0.0658
		b.	0.1514	0.0523	0.0389	0.0588	0.0395	0.1077
32	GeXIX	a.	0.1030	0.0392	0.0228	0.0442	0.0451	0.0619
		b.	0.1496	0.0518	0.0385	0.0579	0.0392	0.1060
33	AsXX	a.	0.1016	0.0389	0.0223	0.0435	0.0462	0.0582
		b.	0.1496	0.0519	0.0386	0.0577	0.0392	0.1056
34	SeXXI	a.	0.1004	0.0387	0.0219	0.0429	0.0472	0.0548
		b.	0.1486	0.0517	0.0385	0.0571	0.0391	0.1046
35	BrXXII	a.	0.0993	0.0385	0.0216	0.0424	0.0481	0.0516
		b.	0.1511	0.0526	0.0392	0.0581	0.0398	0.1063
36	KrXXIII	a.	0.0982	0.0383	0.0213	0.0419	0.0489	0.0487
		b.	0.1477	0.0516	0.0384	0.0565	0.0390	0.1033
37	RbXXIV	a.	0.0972	0.0382	0.0211	0.0414	0.0496	0.0461
		b.	0.1353	0.0476	0.0354	0.0509	0.0360	0.0933
38	SrXXV	a.	0.0962	0.0381	0.0208	0.0409	0.0503	0.0437
		b.	0.1338	0.0472	0.0351	0.0502	0.0357	0.0918

Table 1. continued

Z	ION	M	$^3P_0 - ^3P_1$	$^3P_1 - ^3P_0$	$^3P_1 - ^3P_1$	$^3P_1 - ^3P_2$	$^3P_2 - ^3P_1$	$^3P_2 - ^3P_2$
39	YXXVI	a	0.0953	0.0380	0.0207	0.0405	0.0508	0.0416
		b	0.1388	0.0490	0.0365	0.0523	0.0370	0.0956
40	ZrXXVII	a	0.0944	0.0380	0.0205	0.0400	0.0514	0.0397
		b	0.1473	0.0518	0.0387	0.0560	0.0391	0.1023
41	NbXXVIII	a	0.0936	0.0380	0.0204	0.0396	0.0519	0.0380
		b	0.1481	0.0521	0.0389	0.0563	0.0394	0.1027
42	MoXXIX	a	0.0928	0.0380	0.0203	0.0393	0.0524	0.0365
		b	0.1478	0.0521	0.0389	0.0554	0.0393	0.1010
44	RuXXXI	a	0.0914	0.0382	0.0202	0.0386	0.0534	0.0339
		b	0.1213	0.0436	0.0325	0.0435	0.0330	0.0795
45	RhXXXII	a	0.0907	0.0383	0.0201	0.0383	0.0538	0.0328
		b	0.1220	0.0439	0.0328	0.0435	0.0332	0.0794
46	PdXXXIII	a	0.0900	0.0384	0.0201	0.0380	0.0543	0.0318
		b	0.1239	0.0446	0.0333	0.0439	0.0337	0.0802
47	AgXXXIV	a	0.0894	0.0385	0.0201	0.0377	0.0547	0.0309
		b	0.1280	0.0458	0.0342	0.0450	0.0347	0.0821
48	CdXXXV	a	0.0887	0.0387	0.0202	0.0374	0.0552	0.0301
		b	0.1312	0.0471	0.0352	0.0463	0.0355	0.0842
49	InXXXVI	a	0.0882	0.0389	0.0202	0.0372	0.0557	0.0294
50	SnXXXVII	a	0.0876	0.0391	0.0202	0.0369	0.0562	0.0287
51	SbXXXVIII	a	0.0870	0.0393	0.0203	0.0367	0.0567	0.0281
52	TeXXXIX	a	0.0865	0.0395	0.0204	0.0364	0.0572	0.0275
53	IXL	a	0.0860	0.0398	0.0205	0.0362	0.0577	0.0270
54	XeXLI	a	0.0855	0.0401	0.0206	0.0360	0.0583	0.0265

transitions are those corresponding to $\Delta J = \Delta L$, in the two groups of triplet-triplet transitions which correspond, respectively, to the first three and last three columns of the table.

In Table 2, we compare our two sets of f -values for the $3s^2 3p^2 \ ^1D_2 - 3s^2 3p^1 4s^1 \ ^1P_1$ transition with a few theoretical results, which seem to be the only data available in the literature. For the first four ions, it is possible to compare our oscillator strengths with data reported by Biémont, using the same HXR method as in the above transition (Biémont 1986a), and with the f -values obtained with the length and velocity forms of the dipole transition operator by Nahar & Pradhan (1993) within the Opacity Project. Their method of calculation, the close coupling (CC) approximation using the R-matrix method, explicitly accounts for configuration interaction. For these ions, our f -values appear to be in general good agreement with the other theoretical results, again expected to be correct. For the last several ions we have used the energies obtained in our MCDF calculations for extracting quantum defects to be used in RQDO procedure. This has led to no breakage in the steadily decreasing trend of the RQDO f -values

with increasing Z , which can be taken as a sign of consistency of the RQDO procedure. One possible feature that may explain the discrepancies between the RQDO oscillator strengths and those obtained by Biémont (1986a) (which are, in no case, greater than 8%) is his reported perturbations between the $3s^1 3p^3$ and $3s^2 3p^1 ns^1$ configurations, which have a non-negligible influence on the $3s^2 3p^2 \ ^1D_2 - 3s^2 3p^1 4s^1 \ ^1P_1$ transition probabilities. The mixing between the 3P and 1P terms of the $3s^2 3p^1 4s^1$ configuration, as detected by Biémont (1986a) from his analysis of the energy data (Corliss & Sugar 1979a, b; Sugar & Corliss 1979, 1980) may also be responsible for the aforementioned discrepancies.

In Table 3 we include only our RQDO f -values given that an extense MCDF calculation, using Declaux's code (1975), has been reported by Huang (1985). For the $3s^2 3p^2 \ ^1D_2 - 3s^2 3p^1 3d^1 \ ^1D_2$ transition, our RQDO results, which explicitly account for core polarization effects, are close in magnitude to the HXR f -values reported by Biémont (1986a, b), by Bromage (1980) and Bromage et al. (1978), as well as other theoretical values, which are claimed by their authors to be correct.

Table 2. Oscillator strengths for the transition $3s^2 3p^2 \ ^1D_2 - 3s^2 3p^1 4s^1 \ ^1P_1$

Z	ION	RQDO ^a	MCDF ^b	Other theoretical values
19	KVI	0.1348	0.1401	0.1384 ^c
20	CaVII	0.1258	0.1357	0.1321 ^c , 0.141 – 0.137 ^d
21	ScVIII	0.1180	0.1309	0.1291 ^c
22	TiIX	0.1113	0.1262	0.1205 ^c
23	VX	0.1117	0.1217	
24	CrXI	0.1068	0.1174	
25	MnXII	-	0.1133	
26	FeXIII	0.0976	0.1094	
27	CoXIV	0.0937	0.1057	
28	NiXV	0.0911	0.1021	
29	CuXVI	0.0860	0.0986	
30	ZnXVII	0.0803	0.0952	
31	GaXVIII	0.0720	0.0919	
32	GeXIX	0.0697	0.0888	
33	AsXX	0.0691	0.0858	
34	SeXXI	0.0676	0.0830	
35	BrXXII	0.0697	0.0804	
36	KrXXIII	0.0660	0.0781	
37	RbXXIV	0.0523	0.0760	
38	SrXXV	0.0478	0.0742	
39	YXXVI	0.0436	0.0725	
40	ZrXXVII	0.0399	0.0711	
41	NbXXVIII	0.0366	0.0698	
42	MoXXIX	0.0335	0.0688	
44	RuXXXI	0.0288	0.0670	
45	RhXXXII	0.0267	0.0664	
46	PdXXXIII	0.0249	0.0659	
47	AgXXXIV	0.0234	0.0654	
48	CdXXXV	0.0220	0.0651	
49	InXXXVI	0.0232	0.0648	
50	SnXXXVII	0.0179	0.0647	
51	SbXXXVIII	0.0190	0.0646	
52	TeXXXIX	0.0182	0.0645	
53	IXL	0.0175	0.0646	
54	XeXLI	0.0165	0.0647	

- a) RQDO with polarization, this work.
b) MCDF, this work.
c) HXR (Biémont 1986a).
d) O.P., length and velocity forms, respectively (Nahar & Pradhan 1993).

However, the MCDF f -values from Huang (1985) show very large discrepancies with the rest of the theoretical results displayed in Table 3. These discrepancies increase with atomic number, being the MCDF oscillator strengths too small. When comparing these MCDF data with those of our own MCDF calculations (not shown in the Table 3), the latter present the same feature roughly the same characteristics as Huang's (1985). This leads us to suggest that the MCDF procedure is not adequate for this particular transition, possibly due to cancellation effects in the transition integral. Biémont (1986b) also attributes the large discrepancies observed between Huang's f -values and his HXR f -values to an incorrect assignment of the $3s^2 3p^1 3d^1 \ ^1D_2$ energy levels by Huang (1985). We once more explain the much less important discrepancies observed between the RQDO oscillator strengths and the HXR ones (Biémont 1986a, b) to their explicit inclusion of configuration mixing. This seems to be particularly

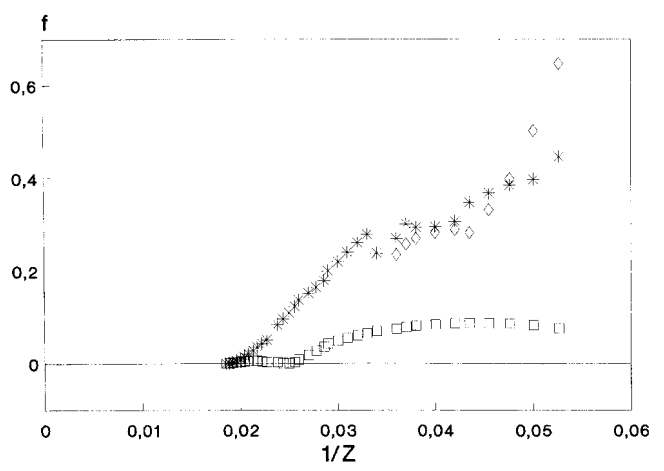


Fig. 1. Oscillator strengths versus the reciprocal of the nuclear charge for the $3s^2 3p^2 \ ^1D_2 \rightarrow 3s^2 3p^1 3d^1 \ ^1D_2$ transition in the silicon isoelectronic sequence. *: RQDO, this work. \square : MCDF, Huang (1985). \diamond : HXR, Biémont (1986a, b)

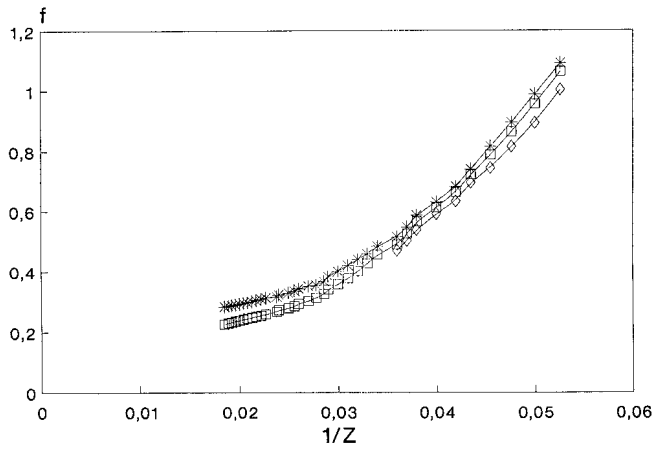


Fig. 2. Systematic trends of the oscillator strength of the $3s^2 3p^2 \ ^1D_2 \rightarrow 3s^2 3p^1 3d^1 \ ^1F_3$ transition along the silicon isoelectronic sequence. *: RQDO, this work. \square : MCDF, Huang (1985). \diamond : HXR, Biémont (1986a, b)

important between $\ ^1D_2$ level corresponding to the final $3s^2 3p^1 3d^1$ state, and the $3s^1 3p^3 \ ^1P_1$ level and more so as Z increases (Biémont 1986a), as in the previous transition.

For the singlet-singlet $3s^2 3p^2 \ ^1D_2 - 3s^2 3p^1 3d^1 \ ^1F_3$ transition, we have calculated oscillator strengths using our semiempirical procedure RQDO only. In Table 3 our f -values are compared with other theoretical results. The most extensive calculation is the MCDF one performed by Huang (1985). This author has accounted for electron correlation by including all relativistic configurations in the $n = 3$ complex. Our semiempirical f -values are in better agreement than in previous transitions with the values obtained with the quite much more complex procedures, even with the results obtained using the ample

Table 3. Oscillator strengths for the transitions involving the metaestable level 1D_2 , $3s^2 3p^2 ^1D_2 - 3s^2 3p^1 3d^1 ^1D_2$ and $3s^2 3p^2 ^1D_2 - 3s^2 3p^1 3d^1 ^1F_3$

Z	ION	$^1D_2 - ^1D_2$			$^1D_2 - ^1F_3$		
		RQDO ^a	MCDF ^b	others	RQDO ^a	MCDF ^b	others
19	KVI	0.4467	0.0762	0.6472 ^c	1.0901	1.061	1.0024 ^c
20	CaVII	0.3977	0.0826	0.5024 ^c 0.678/0.674 ^d	0.9873	0.9549	0.8934 ^c
21	ScVIII	0.3850	0.0862	0.3991 ^c	0.8956	0.8640	0.8148 ^c
22	TiIX	0.3679	0.0876	0.3319 ^c	0.8160	0.7864	0.7431 ^c
23	VX	0.3480	0.0874	0.2825 ^e 0.266 ^f	0.7385	0.7197	0.6935 ^e 0.744 ^f
24	CrXI	0.3067	0.0861	0.2891 ^e	0.6809	0.6617	0.6325 ^e
25	MnXII	0.2948	0.0839	0.2825 ^e	0.6297	0.6106	0.5902 ^e
26	FeXIII	0.2935	0.0810	0.2698 ^e 0.268 ^g 0.2761 ^h	0.5862	0.5652	0.5383 ^e 0.582 ^g 0.5768 ⁱ
27	CoXIV	0.3008	0.0775	0.2576 ^e	0.5474	0.5244	0.5024 ^e
28	NiXV	0.2692	0.0735	0.2350 ^e 0.20 ^f	0.5143	0.4878	0.4688 ^e 0.51 ^f
29	CuXVI	0.2375	0.0691		0.4840	0.4547	
30	ZnXVII	0.2781	0.0644		0.4578	0.4251	
31	GaXVIII	0.2603	0.0593		0.4398	0.3988	
32	GeXIX	0.2398	0.0540		0.4194	0.3756	
33	AsXX	0.2189	0.0462		0.3998	0.3555	
34	SeXXI	0.1991	0.0419		0.3831	0.3382	
35	BrXXII	0.1775	0.0348		0.3654	0.3234	
36	KrXXIII	0.1635	0.0267		0.3532	0.3109	
37	RbXXIV	0.1511	0.0175		0.3505	0.3002	
38	SrXXV	0.1362	0.0083		0.3419	0.2912	
39	YXXVI	0.1224	0.0021		0.3340	0.2836	
40	ZrXXVII	0.1087	6.05(-5)		0.3271	0.2770	
41	NbXXVIII	0.0956	0.0004		0.3208	0.2713	
42	MoXXIX	0.0834	0.0016		0.3151	0.2662	
44	RuXXXI	0.0512	0.0041		0.3115	0.2576	
45	RhXXXII	0.0428	0.0048		0.3070	0.2537	
46	PdXXXIII	0.0349	0.0050		0.3029	0.2501	
47	AgXXXIV	0.0274	0.0048		0.2993	0.2466	
48	CdXXXV	0.0209	0.0041		0.2960	0.2433	
49	InXXXVI	0.0148	0.0031		0.2931	0.2401	
50	SnXXXVII	0.0095	0.0020		0.2905	0.2370	
51	SbXXXVIII	0.0054	0.0011		0.2882	0.2339	
52	TeXXXIX	0.0023	4.44(-4)		0.2863	0.2309	
53	IXL	0.0004	1.15(-4)		0.2846	0.2280	
54	XeXLI	0.0000	2.24(-6)		0.2832	0.2252	

a) RQDO, this work; b) MCDF (Huang 1985); c) HXR (Biémont 1986a); d) O.P., $f_{\text{length}}/f_{\text{velocity}}$ (Nahar & Pradhan 1993); e) HXR (Biémont 1986b); f) HXR (Bromage 1980); g) HXR (Bromage et al. 1978); h) Flower & Nussbaumer (1974); i) Fuhr et al. (1981).

Multiconfigurational Dirac-Fock method, possibly due to the less delicate level perturbation situation here.

Finally, in Figs. 1 and 2 we compare the oscillator strengths corresponding to the last two transitions, respectively, in graph form. For that purpose, we have plotted the f -value for the entire group of isoelectronic ions against the reciprocal of the atomic number Z . These figures also serve the purpose of reflecting systematic trends in the individual f -values along the isoelectronic sequence, which have long been considered (Wiese & Weiss 1968) as a qualitative proof of correctness and allows, when they are regular enough, the interpolation or extrapolation of non-calculated data.

4. Concluding remarks

The RQDO oscillator strengths calculated for the $3s^2 3p^2 ^1D_2 - 3s^2 3p^1 4s^1 ^1P_1$, $3s^2 3p^2 ^1D_2 - 3s^2 3p^1 3d^1 ^1F_3$, $3s^2 3p^2 ^1D_2 - 3s^2 3p^1 3d^1 ^1D_2$, and $3s^2 3p^2 ^3P - 3s^2 3p^1 4s^1 ^3P$ transitions in the silicon isoelectronic sequence are in reasonable general agreement with the results of the rather more sophisticated MCDF calculations, which account for inner and outer correlation, and for relativistic effects, as well as with a few theoretical data found in the literature for the individual lines. An independent proof of the reliability of our RQDO results except for the very highly charged ions is the correct systematic trends followed by most of our line f -values.

Overall, we seem to find reasons to be hopeful about the possibilities offered by the RQDO formalism

for predicting spectral properties of many-valence electron atomic systems which are of interest in astrophysics and nuclear fusion research, whenever the complications brought about by the presence of configuration interaction are not too severe. One attractive feature of the RQDO formalism is its analyticity, which implies low computational expense and avoidance of the numerous convergence problems which are common in the MCDF approach.

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