

# Relativistic quantum defect orbital calculations of oscillator strengths in neutral chlorine

C. Lavín, A.M. Velasco, and I. Martín

Departamento de Química Física, Facultad de Ciencias, E-47005 Valladolid, Spain

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**Abstract.** The Relativistic Quantum Defect Orbital (RQDO) method without and with explicit inclusion of core polarization has been applied to the study of oscillator strengths of fine structure transitions in neutral chlorine, some of which are important in interstellar chemistry. The resulting oscillator strengths are analyzed in terms of other theoretical results and some available experimental data. For the  $3p^4(^3P)4f - 3p^4(^3P)5g$  lines we supply the only available results at the moment.

**Key words:** atomic data – ISM: atoms

## 1. Introduction

Models of interstellar chlorine chemistry can be used to constrain models of interstellar clouds (Jura 1974, Jura & York 1978). Since  $H_2$  is abundant in virtually all interstellar clouds (Spitzer et al. 1973), ion-molecule reactions of the form  $X^+ + H_2 \rightarrow XH^+ + H$  can dominate the cloud chemistry (Black & Dalgarno 1973; Herbst & Klemperer 1973; Watson 1973). Most atoms that are normally ionized in regions primarily composed of atomic hydrogen cannot react exothermically with thermal  $H_2$  (Dalgarno et al. 1974); however chlorine is exceptional. Because of the rapid reaction of  $Cl^+$  with  $H_2$ , it is expected that in regions where the hydrogen is primarily atomic, chlorine is ionized; in regions where there is a significant amount of molecular hydrogen, chlorine is neutral. One difficulty to confirm the basic ideas of this model is that the analyses have been based on rather poorly known oscillator strengths for  $Cl I$ , as has been emphasized by Keenan & Dufton (1990) and Morton (1991).

In previous calculations (Velasco et al. 1997) of oscillator strengths in neutral fluorine, we have followed a semiempirical procedure, the quasirelativistic Quantum Defect Orbital (RQDO) method. Given the satisfactory results obtained for this atom, we have now extended our calculations of oscillator strengths to several fine structure transitions in neutral chlorine.

*Send offprint requests to:* C. Lavín. Phone +34-83-423481. Fax +34-83-423013. e-mail: clavin@cpd.uva.es

We have followed the RQDO procedure with and without explicit inclusion of core-valence correlation. The observations (Radziemski & Kaufman 1969) of the  $Cl I$  spectrum show that LS coupling is valid for the deepest  $3p^4 ns, np$  and  $nd$  configurations whereas pair coupling is progressively better satisfied for higher  $l$  and  $n$  values. In our calculations of oscillator strengths we have followed the LS coupling scheme, except for the  $3p^4(^3P)4f - 3p^4(^3P)5g$  lines, for which the  $J_c l$  coupling scheme seems clearly to be more appropriate.

The neutral chlorine lines at  $1097\text{\AA}(3p^5\ ^2P_{3/2}^0 - 3p^4(^3P)3d\ ^2D_{5/2})$  and  $1347\text{\AA}(3p^5\ ^2P_{3/2}^0 - 3p^4(^3P)4s\ ^2P_{3/2})$  are of interest in the study of interstellar matter. Schectman et al. (1993) have measured the lifetimes and deduced the oscillator strengths for the above lines using beam-foil spectroscopy. Their result for  $\lambda 1347$  is the most accurate laboratory datum available and it is somewhat larger than earlier determinations. These authors suggest that, provided that their value differs from the values used in previous studies of chlorine in diffuse interstellar clouds, the chemical picture that emerged from those studies needs to be reexamined. Our  $f$  value for the line at 1347 confirms the result of Schectman et al. (1993).

## 2. Method of calculation

The relativistic quantum defect orbitals corresponding to a state characterized by its experimental energy  $E^x$  are the analytical solutions of the quasirelativistic second-order Dirac-like equation (Martin & Karwowski 1991; Karwowski & Martin 1991)

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

where the parameter  $\Lambda$ , which accounts for polarization and penetration effects of the valence electron, is related to the relativistic principal quantum number  $\tilde{n}$ , the principal and orbital angular momentum quantum numbers,  $n$  and  $l$ , respectively, the relativistic quantum defect,  $\delta'$ , and an integer,  $c$ , chosen to ensure the normalizability of the wavefunction and its correct nodal structure

$$\Lambda = \tilde{n} - n + l - \delta' + c, \quad (2)$$

**Table 1.** Oscillator strengths for the  $3p^5 - 3p^4(^3P)4s$  fine structure transitions in  $Cl I$ 

	RQDO <sup>a</sup>	RQDO <sup>b</sup>	SST <sup>c</sup>	CIV3 <sup>d</sup>	CC <sup>e</sup>	Experiment
$3p^2P_{3/2}^0 - 4s^2P_{3/2}$	0.1368	0.1281	0.147	0.1324	0.114	0.100±0.030 <sup>f</sup> 0.109±0.010 <sup>g</sup> 0.153±0.011 <sup>h</sup>
$3p^2P_{3/2}^0 - 4s^2P_{1/2}$	0.0249	0.0240	0.0299	0.0264	0.0233	0.028±0.006 <sup>f</sup>
$3p^2P_{1/2}^0 - 4s^2P_{3/2}$	0.0561	0.0523	0.0530	0.0474	0.0418	0.038±0.006 <sup>f</sup> 0.055±0.004 <sup>h</sup>
$3p^2P_{1/2}^0 - 4s^2P_{1/2}$	0.1017	0.0980	0.116	0.1051	0.088	0.093±0.016 <sup>f</sup>

<sup>a</sup> RQDO without explicit polarization correction, this work<sup>b</sup> RQDO with explicit polarization correction, this work<sup>c</sup> Biémont et al. (1994), length form<sup>d</sup> Ojha & Hibbert (1990), length form<sup>e</sup> Critical compilation, Wiese et al. (1969)<sup>f</sup> Clyne & Nipp (1976)<sup>g</sup> Schwab & Anderson (1982)<sup>h</sup> Schectman et al. (1993)**Table 2.** Oscillator strengths for the  $3p^5 - 3p^4(^3P)3d$  fine structure transitions in  $Cl I$ 

Transition	RQDO <sup>a</sup>	RQDO <sup>b</sup>	SST( $f_l$ ) <sup>c</sup>	SST( $f_v$ ) <sup>c</sup>	CIV3( $f_l$ ) <sup>d</sup>	CIV3( $f_v$ ) <sup>d</sup>	Expt <sup>f</sup>
$3p^2P_{3/2}^0 - 3d^2P_{3/2}$	0.0228	0.0170	0.0320	0.0303	0.0111	0.0052	
$3p^2P_{3/2}^0 - 3d^2P_{1/2}$	0.0057	0.0041	0.0018	0.0009	0.0046	0.0018	
$3p^2P_{1/2}^0 - 3d^2P_{3/2}$	0.0093	0.0070	0.0151	0.0140	0.0432	0.0182	
$3p^2P_{1/2}^0 - 3d^2P_{1/2}$	0.0228	0.0170	0.0124	0.0097	0.0176	0.0065	
$3p^2P_{3/2}^0 - 3d^2D_{5/2}$	0.1032	0.0757	0.0803	0.0730	0.0423	0.0170	0.0088
$3p^2P_{3/2}^0 - 3d^2D_{3/2}$	0.0114	0.0083	0.0109	0.0083	0.0134	0.0053	
$3p^2P_{1/2}^0 - 3d^2D_{3/2}$	0.1161	0.0852	0.0128	0.0130	0.0367	0.0152	

<sup>a</sup> RQDO without explicit polarization correction, this work<sup>b</sup> RQDO with explicit polarization correction, this work<sup>c</sup> Biémont et al. (1994), length and velocity forms<sup>d</sup> Ojha & Hibbert (1990), length and velocity forms<sup>f</sup> Schectman et al. (1993), ± 0.0013 error bar

$Z'_{net}$  is the scaled  $Z_{net}$ , the screened nuclear charge at large radial distances,

$$Z'_{net} = Z_{net}(1 + \alpha^2 E^x), \quad (3)$$

with  $\alpha$  being the fine-structure constant. To determine the relativistic quantum defect, the following expression is employed,

$$e^{RD} = -\frac{(Z'_{net})^2}{2(\tilde{n} - \delta')^2} = E^x \frac{(1 + \alpha^2 E^x/2)}{(1 + \alpha^2 E^x)^2}. \quad (4)$$

Once  $\delta'$  is known, the model potential parameter  $\Lambda$  is obtained from Eq. (2) and substituted into Eq. (1), which can be solved analytically. Since the effective Hamiltonian in Eq. (1) includes a screening term, the quantum defect orbitals are approximately valid in the core region of space. 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.

As previously done (Lavín et al. 1993), we have employed two different forms of the transition operator,  $Q(r)=r$ , and a core-polarization corrected expression (Bielińska-Wąz 1992), given by:

$$Q(r) = r \left\{ 1 - \frac{\alpha_c}{r^3} [1 - \exp(-r/r_c)]^3 \right\} \quad (5)$$

where  $\alpha_c$  is the core-polarizability and  $r_c$  is a cutoff radius.

The inclusion of a core-polarization correction in the computation of transition probabilities for atomic systems has long been considered important. The model potential parameter given by Eq. (2) implicitly accounts for core-valence correlation, also known as core-valence polarization. This partly avoids the addition of a core-polarization term to the model potential, depending on free parameters. Laughlin (1989) has pointed out that when matrix elements are calculated with wave functions obtained from a valence electron Schrödinger equation, core-polarization corrections introduced in the transition operator are especially adequate.

We have carried out calculations for transitions for which empirical energy data were available (Radziemski & Kaufman 1969). The core polarizabilities have been taken 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).

### 3. Results

In Tables 1–5, we report oscillator strengths for  $3p^5 - 3p^4(^3P)4s$ ,  $3p^5 - 3p^4(^3P)3d$ ,  $3p^4(^3P)4s - 3p^4(^3P)4p$ ,  $3p^4(^3P)4p - 3p^4(^3P)5s$ , and  $3p^4(^3P)4f - 3p^4(^3P)5g$ , fine structure transitions in neutral chlorine. Two sets of RQDO  $f$ -values are shown, those computed with the standard dipole length oper-

**Table 3.** Oscillator strengths for the  $3p^4(^3P)4s - 3p^4(^3P)4p$  fine structure transitions in *Cl I*

Transition	RQDO <sup>a</sup>	RQDO <sup>b</sup>	CIV3(f <sub>l</sub> ) <sup>c</sup>	CIV3(f <sub>v</sub> ) <sup>c</sup>	CC <sup>d</sup>	Expt <sup>e</sup>
$4s^2P_{3/2} - 4p^2S_{1/2}^0$	0.1051	0.0994	0.0098	0.0113	0.12	
$4s^2P_{1/2} - 4p^2S_{1/2}^0$	0.1061	0.1003	0.3517	0.3195	0.12	
$4s^2P_{3/2} - 4p^2P_{3/2}^0$	0.2622	0.2471	0.0970	0.0768		
$4s^2P_{3/2} - 4p^2P_{1/2}^0$	0.0523	0.0492	0.1726	0.1595		0.0103
$4s^2P_{1/2} - 4p^2P_{3/2}^0$	0.1053	0.0996	0.4269	0.3982		
$4s^2P_{1/2} - 4p^2P_{1/2}^0$	0.2096	0.1917	0.0265	0.0193		
$4s^2P_{3/2} - 4p^2D_{5/2}^0$	0.4632	0.4337	0.4106	0.4010	0.50	
$4s^2P_{3/2} - 4p^2D_{3/2}^0$	0.0520	0.0488	0.2202	0.1979	0.057	
$4s^2P_{1/2} - 4p^2D_{3/2}^0$	0.5195	0.4875	0.2081	0.2200	0.56	
$4s^4P_{5/2} - 4p^4P_{5/2}^0$	0.2053	0.1895	0.3355	0.2701	0.22	
$4s^4P_{5/2} - 4p^4P_{3/2}^0$	0.0887	0.0821	0.1636	0.1307	0.095	
$4s^4P_{3/2} - 4p^4P_{5/2}^0$	0.1311	0.1210	0.0870	0.0727	0.14	
$4s^4P_{3/2} - 4p^4P_{3/2}^0$	0.0392	0.0363	0.0629	0.0516	0.042	
$4s^4P_{3/2} - 4p^4P_{1/2}^0$	0.1239	0.1148	0.1773	0.1442	0.13	
$4s^4P_{1/2} - 4p^4P_{3/2}^0$	0.2441	0.2258	0.1683	0.1415	0.26	
$4s^4P_{1/2} - 4p^4P_{1/2}^0$	0.0494	0.0458	0.0371	0.0301	0.052	
$4s^4P_{5/2} - 4p^4S_{3/2}^0$	0.0996	0.0944	0.0772	0.0555	0.10	0.0800
$4s^4P_{3/2} - 4p^4S_{3/2}^0$	0.1012	0.0958	0.1169	0.0846	0.11	0.103
$4s^4P_{1/2} - 4p^4S_{3/2}^0$	0.1021	0.0966	0.1722	0.1266	0.12	0.11
$4s^4P_{5/2} - 4p^4D_{7/2}^0$	0.4032	0.3754	0.5392	0.4092	0.39	
$4s^4P_{5/2} - 4p^4D_{5/2}^0$	0.0911	0.0850	0.0468	0.0351	0.080	0.056
$4s^4P_{5/2} - 4p^4D_{3/2}^0$	0.0102	0.0095	0.0006	0.0040	0.010	
$4s^4P_{3/2} - 4p^4D_{5/2}^0$	0.3197	0.2982	0.3818	0.2987	0.31	1.6
$4s^4P_{3/2} - 4p^4D_{3/2}^0$	0.1633	0.1528	0.1799	0.1374	0.16	0.093
$4s^4P_{3/2} - 4p^4D_{1/2}^0$	0.0256	0.0240	0.0189	0.0143	0.025	0.021
$4s^4P_{1/2} - 4p^4D_{3/2}^0$	0.2559	0.2394	0.3540	0.2750	0.27	0.251
$4s^4P_{1/2} - 4p^4D_{1/2}^0$	0.2566	0.2405	0.3592	0.2752	0.25	0.202

<sup>a</sup> RQDO without explicit polarization correction, this work<sup>b</sup> RQDO with explicit polarization correction, this work<sup>c</sup> Ojha & Hibbert (1990), length and velocity forms<sup>d</sup> Critical compilation, Wiese et al. (1969)<sup>e</sup> Bengtson et al. (1971)

ator,  $Q(r)=r$ , and those where core-valence correlation has been explicitly introduced, Eq. (5). Other oscillator strengths, from theoretical calculations and experiment found in the literature, have been included in the tables for a comparative analysis. Comparison between theory and experiment remains an important tool for assessing the accuracy of calculations and probably as important is the comparison with other independent calculations, as pointed out recently by Hibbert (1996).

### 3.1. $3p^5\ ^2P^0 - 3p^4(^3P)4s\ ^2P$ transitions

Some lines of the  $3p^5\ ^2P^0 - 3p^4(^3P)4s\ ^2P$  multiplet of neutral chlorine have been the object of several theoretical studies, as well as measurements because of their importance in astrophysics. Table 1 contains fine structure oscillator strengths for the  $3p^5\ ^2P^0 - 3p^4(^3P)4s\ ^2P$  transitions in *Cl I*. In this table we display, together with the RQDO results, the f-values calculated by Biémont et al. (1994) with the SUPERSTRUCTURE (SST) computer program, taking the most important configuration interaction and relativistic effects into account and results of Ojha & Hibbert (1990), who used large multiconfiguration

expansions in the atomic structure code CIV3. Biémont et al. and Ojha & Hibbert report f-values calculated in dipole length and velocity approaches. In both CIV3 and SST calculations, the length and velocity f-values are close to each other in magnitude. For this reason, and in order not to make Table 1 excessively broad, we have only included the length values of both procedures. An indicator (though not a guarantee) of accuracy of f-values is the extent of the agreement between both forms of oscillator strengths. On this basis, Biémont et al. claim that their results are the most accurate theoretical data available for these transitions.

The experimental data found in the literature are also shown in the table. Earlier measurements of these transitions have been carried out by Hoffman (1967) who used a wall-stabilized arc as a light source and by Lawrence (1967) who measured the f value for the  $3p^5\ ^2P_{3/2}^0 - 3p^44s\ ^2P_{1/2}$  line using the phase-shift method and did an intermediate coupling calculation of the transition strengths for the other lines. The literature evaluations of Wiese et al. (1969) based on the cited work of Hoffman and Lawrence are tabulated. Clyne & Nipp (1977) measured

**Table 4.** Oscillator strengths for the  $3p^4(^3P)4p - 3p^4(^3P)5s$  fine structure transitions in  $Cl I$ 

Transition	RQDO <sup>a</sup>	RQDO <sup>b</sup>	CIV3( $f_i$ ) <sup>c</sup>	CIV3( $f_v$ ) <sup>c</sup>
$4p^4S_{3/2}^0 - 5s^4P_{5/2}$	0.1556	0.1542	0.1264	0.0995
$4p^4S_{3/2}^0 - 5s^4P_{3/2}$	0.1023	0.1015	0.1006	0.0604
$4p^4S_{3/2}^0 - 5s^4P_{1/2}$	0.0488	0.0487	0.0212	0.0087
$4p^4P_{5/2}^0 - 5s^4P_{5/2}$	0.1804	0.1804	0.1931	0.0500
$4p^4P_{5/2}^0 - 5s^4P_{3/2}$	0.0718	0.0712	0.0157	0.0038
$4p^4P_{5/2}^0 - 5s^4P_{1/2}$	0.1184	0.1183	0.1372	0.0374
$4p^4P_{3/2}^0 - 5s^4P_{3/2}$	0.0327	0.0328	0.0130	0.0030
$4p^4P_{3/2}^0 - 5s^4P_{1/2}$	0.0902	0.0911	0.0706	0.0195
$4p^4P_{1/2}^0 - 5s^4P_{3/2}$	0.2102	0.2106	0.0940	0.0251
$4p^4P_{1/2}^0 - 5s^4P_{1/2}$	0.0373	0.0376	0.0277	0.0079
$4p^4D_{7/2}^0 - 5s^4P_{5/2}$	0.2819	0.2807	0.2641	0.0981
$4p^4D_{7/2}^0 - 5s^4P_{3/2}$	0.0861	0.0857	0.0292	0.0115
$4p^4D_{7/2}^0 - 5s^4P_{1/2}$	0.1912	0.1909	0.0051	0.0008
$4p^4D_{5/2}^0 - 5s^4P_{5/2}$	0.0147	0.0146	0.0005	0.0002
$4p^4D_{5/2}^0 - 5s^4P_{3/2}$	0.1504	0.1500	0.0097	0.0022
$4p^4D_{5/2}^0 - 5s^4P_{1/2}$	0.1078	0.1081	0.1288	0.0465
$4p^4D_{3/2}^0 - 5s^4P_{3/2}$	0.0478	0.0476	0.0264	0.0007
$4p^4D_{3/2}^0 - 5s^4P_{1/2}$	0.2207	0.2210	0.2162	0.0894
$4p^2D_{5/2}^0 - 5s^2P_{3/2}$	0.2859	0.2849	0.0083	0.0061
$4p^2D_{3/2}^0 - 5s^2P_{3/2}$	0.0489	0.0487	0.0431	0.0294
$4p^2D_{3/2}^0 - 5s^2P_{1/2}$	0.2468	0.2453	0.0909	0.0377
$4p^2P_{3/2}^0 - 5s^2P_{3/2}$	0.2518	0.2502	0.0395	0.0227
$4p^2P_{3/2}^0 - 5s^2P_{1/2}$	0.0507	0.0503	0.1028	0.0533
$4p^2P_{1/2}^0 - 5s^2P_{3/2}$	0.0995	0.0990	0.0441	0.0259
$4p^2P_{1/2}^0 - 5s^2P_{1/2}$	0.2006	0.1992	0.0264	0.0138

<sup>a</sup> RQDO without explicit polarization correction, this work<sup>b</sup> RQDO with explicit polarization correction, this work<sup>c</sup> Ojha & Hibbert (1990), length and velocity forms

$f$  values by resonance absorption and obtained a precision of some 30%. An improvement to the experiment of Clyne & Nipp was carried out by Schwab & Anderson (1982) who quoted 10% accuracy. The most accurate laboratory data are the measurements of Schectman et al. (1993) by using beam-foil spectroscopy. These authors estimated that their results should be accurate to about 7%. The present results without explicit account for polarization are in good accordance with the most accurate theoretical and experimental results. Our  $f$ -values for the  $3p^5\ ^2P_{3/2}^0 - 3p^4(^3P)4s\ ^2P_{3/2}$  and  $3p^5\ ^2P_{1/2}^0 - 3p^4(^3P)4s\ ^2P_{3/2}$  lines are larger than the earlier measurements for these transitions, and confirm the recent experimental data of Schectman et al. For the remaining transitions, our  $f$ -values are in good accord with the measurements of Clyne & Nipp (1976).

### 3.2. $3p^5 - 3p^4(^3P)3d$ transitions

In Table 2 we display, together with the RQDO results, the SST  $f$ -values calculated by Biémont et al. (1994) and the CIV3 results by Ojha & Hibbert (1990). The only experimental data for these transitions is due to Schectman et al. (1993). As emphasized by Schectman et al., the  $3p^4(^3P)3d$  configuration mixes with

**Table 5.** Oscillator strengths for the  $3p^4(^3P_2)4f[K]_J - 3p^4(^3P_2)5g[K]_J$  transitions in  $Cl I$ 

	RQDO <sup>a</sup>	RQDO <sup>b</sup>		RQDO <sup>a</sup>	RQDO <sup>b</sup>
$[5]_{11/2} - [6]_{13/2}$	1.2217	1.2211	$[3]_{7/2} - [4]_{9/2}$	1.0697	1.0691
$[5]_{11/2} - [6]_{11/2}$	0.1031	0.1030	$[3]_{7/2} - [4]_{7/2}$	0.0307	0.0306
$[5]_{9/2} - [6]_{11/2}$	1.2354	1.2348	$[3]_{5/2} - [4]_{7/2}$	1.0989	1.0983
$[5]_{11/2} - [5]_{11/2}$	0.1031	0.1030	$[3]_{7/2} - [3]_{7/2}$	0.2247	0.2246
$[5]_{11/2} - [5]_{9/2}$	0.0016	0.0016	$[3]_{7/2} - [3]_{5/2}$	0.0083	0.0083
$[5]_{9/2} - [5]_{11/2}$	0.0019	0.0019	$[3]_{5/2} - [3]_{7/2}$	0.0111	0.0111
$[5]_{9/2} - [5]_{9/2}$	0.1028	0.1027	$[3]_{5/2} - [3]_{5/2}$	0.2220	0.2219
$[5]_{11/2} - [4]_{9/2}$	0.0040	0.0040	$[2]_{5/2} - [3]_{7/2}$	1.0668	1.0662
$[5]_{9/2} - [4]_{9/2}$	0.0001	0.0001	$[2]_{5/2} - [3]_{5/2}$	0.0532	0.0531
$[5]_{9/2} - [4]_{7/2}$	0.0040	0.0039	$[2]_{3/2} - [3]_{5/2}$	1.1201	1.1201
$[4]_{9/2} - [5]_{11/2}$	1.1263	1.1257	$[1]_{3/2} - [2]_{5/2}$	1.1216	1.1209
$[4]_{9/2} - [5]_{9/2}$	0.0209	0.0208	$[1]_{3/2} - [2]_{5/2}$	0.2691	0.2690
$[4]_{7/2} - [5]_{9/2}$	1.1481	1.1475	$[1]_{1/2} - [2]_{3/2}$	1.3466	1.3459
$[4]_{9/2} - [4]_{9/2}$	0.1802	0.1801	$[2]_{5/2} - [2]_{5/2}$	0.2051	0.2050
$[4]_{9/2} - [4]_{7/2}$	0.0041	0.0041	$[2]_{5/2} - [2]_{3/2}$	0.0149	0.0149
$[4]_{7/2} - [4]_{9/2}$	0.0052	0.0052	$[2]_{3/2} - [2]_{5/2}$	0.0224	0.0224
$[4]_{7/2} - [4]_{7/2}$	0.1794	0.1793	$[2]_{3/2} - [2]_{3/2}$	0.0897	0.0897
$[4]_{9/2} - [3]_{7/2}$	0.0093	0.0093			
$[4]_{7/2} - [3]_{5/2}$	0.0089	0.0089			
$[4]_{7/2} - [3]_{7/2}$	0.0004	0.0004			

<sup>a</sup> RQDO without explicit polarization correction, this work<sup>b</sup> RQDO with explicit polarization correction, this work

$3p^4(^3P)5s$  to form a complex of 22 even parity levels. Among these are six levels with  $J=5/2$ . The states with  $J=5/2$  are not well described by LS-coupling or by any other pure coupling scheme, such as  $J_c l$ -coupling. In particular, the level at 91,907  $\text{cm}^{-1}$  has been classified as  $^2D$  by Minnhagen (1961) and as  $^2F$  by Radziemski & Kaufman (1969). Due to the semiempirical nature of the RQDO method, the presently calculated oscillator strengths obviously depend upon the term and level identifications adopted by experimentalists. We used the labelling proposed by Radziemski & Kaufman, but also checked the option of Minnhagen for the  $3p^4(^3P)^2D_{5/2}$  level. The RQDO  $f$ -values for the  $3p^5\ ^2P_{3/2}^0 - 3p^4(^3P)3d\ ^2D_{5/2}$  line obtained with the  $^2D_{5/2}$  energy of Minnhagen are 0.0812 and 0.0604 without and with polarization, respectively. This option would not help improving the agreement between the RQDO results and the beam-foil measurement for this transition. However, the agreement with the results of other theories would be somewhat improved.

### 3.3. $3p^4(^3P)4s - 3p^4(^3P)4p$ transitions

Oscillator strengths for  $3p^4(^3P)4s - 3p^4(^3P)4p$  fine structure transitions are given in Table 3. To analyze the correctness of the  $f$ -values RQDO for these lines comparative theoretical and experimental data have been included in the table. Absolute transition probabilities measured through a gas-driven shock tube with accuracies of 20-40% by Bengtson et al (1971) have been converted into oscillator strengths for comparison. Critically compiled data by Wiese et al. (1969) based on the mea-

surements by Bengtson et al. (1971), and calculations obtained with the Coulomb Approximation are also included in the table. Wiese et al. remark that, for the case of the  $4s^4P - 4p^4D$  multiplet, the stronger lines measured by Bengtson et al. seem to be affected by self-absorption. Table 3 also contains the CIV3 dipole length and dipole velocity oscillator strengths by Ojha & Hibbert (1990). The RQDO results appear to be much closer in magnitude to the recommended  $f$ -values by Wiese et al. than to the CIV3  $f$ -values. On the other hand, the discrepancies between the length and velocity CIV3 oscillator strengths are not negligible.

### 3.4. $3p^4(^3P)4p - 3p^4(^3P)5s$ transitions

In Table 4 we display RQDO  $f$ -values with and without polarization correction for the  $3p^4(^3P)4p - 3p^4(^3P)5s$  fine structure transitions in  $Cl I$ . No experimental  $f$ -values have been found in the literature for these transitions, and our analysis must rest on the comparative theoretical results that are available. The only theoretical  $f$ -values are, to our knowledge, those obtained by Ojha & Hibbert (1990) through CIV3 calculations. For the weaker  $3p^4(^3P)4p - 3p^4(^3P)5s$  transitions, there are larger discrepancies than in previously analyzed transitions between length and velocity CIV3 results.

### 3.5. $3p^4(^3P)4f - 3p^4(^3P)5g$ transitions

Finally, in Table 5 we display RQDO  $f$ -values for  $3p^4(^3P)4f - 3p^4(^3P)5g$  transitions calculated in the  $J_c l$  coupling scheme. No comparative data have been found in the literature. The level designation in Table 5 is given according to the notation  $3p^4(^{2S+1}L_{J_c}nl[K]_J)$  where  $J_c$  is the total angular momentum quantum number of the electron core  $3p^4\ ^3P$  level;  $K$  results from the coupling of the orbital angular momentum  $l$  of the valence electron with  $J_c$ , and  $J$  is obtained through the addition of the spin of the valence electron to  $K$ . According to Quinet et al. (1994), in pure  $J_c l$  coupling, the energies of a pair of levels for a given  $J_c$  should fall on a parabola when plotted against  $h = 1/2[K(K+1) - J_c(J_c+1) - l(l+1)]$ . This approximation is verified in the cases of 4f and 5g electrons.

## 4. Concluding remarks

The RQDO oscillator strengths for the resonance transitions in neutral chlorine are in fairly good agreement with the most accurate theoretical results, that is, those calculated with the SUPERSTRUCTURE computer program, which accounts for configuration interaction and relativistic effects. The RQDO  $f$ -values conform with experimental results and recommended values for the  $3p^4(^3P)4s - 3p^4(^3P)4p$  transitions better than those of the much more complex CIV3 theoretical procedure.

Another feature of the present RQDO results that hints at their correctness is that the effect of the core-polarization correction diminishes as the final state is further away from the core, as it is apparent when comparing the RQDO data of Tables 1 to 5.

Overall, we seem to find reasons to be hopeful about the possibilities of the RQDO formalism for predicting spectral properties of interest in astrophysics. These reasons rest on the correctness of the results so far achieved, and the low computational expense and avoidance of the numerous convergence problems which are common in the multiconfigurational approaches.

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