

# Fine structure levels of Cl V and their lifetimes

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**Abstract.** We report a large scale configuration interaction calculation of Cl V by taking account of relativistic effect through the Breit-Pauli approximation. Excitation energies of the lowest 49 fine structure levels relative to the ground state  $3s^23p(^2P_{1/2}^o)$  are found to be in good agreement with the NIST recommended data. Oscillator strengths, line strengths and radiative rates for the optically allowed and intercombination transitions among these levels and life times for some relatively longer lived fine structure levels are also reported for this ion. We confirm the interesting result that the life times for the multiplets of  $3s3p^2(^4P)$  and  $3s3p(^3P)3d(^4F)$  are of the order of microseconds.

**PACS.** 32.10.Fn Fine and hyperfine structure – 32.70.Cs Oscillator strengths, lifetimes, transition moments – 95.30.Ky Atomic and molecular data, spectra, and spectral parameters (opacities, rotation constants, line identification, oscillator strengths, gf values, transition probabilities, etc.)

## 1 Introduction

Very recently Berrington and Nakazaki [1] reported a comprehensive study of radiative data for neutral chlorine and its ions. They clearly demonstrated the importance and need for further studies on these ions as there are either very few or virtually no data available for ions of Cl. The  $R$ -matrix approach employed by Berrington and Nakazaki [1] is perhaps the only reported detailed study on ions of Cl. Nevertheless, this being an LS coupling calculation will obviously be of limited use in application for diagnostic purpose. One needs at least an intermediate coupling (LSJ) calculation for the dipole allowed and intercombination transitions among various fine structure levels.

Using the *ab initio* package program of Cowan [2], Fawcett [3] calculated wavelengths and oscillator strengths of a few aluminium-like ions including Cl V. This calculation, however, involved configurations only from the  $n = 3$  complex and therefore important CI mixing from the  $n = 4$  for some of the fine-structure levels are ignored. A similar investigation using the Dirac-Fock code of Desclaux [4] was performed by Huang [5] again including some configurations from the  $n = 3$  complex only. Accurate observations on the transitions  $3s^23p(^2P^o) - 3s3p^2(^4P)$  have been reported by Jupen and Curtis [6]. There is virtually no other theoretical calculation for Cl V that include the ef-

fects of a large scale CI mixing as well as some relativistic effects.

Besides the paucity of the radiative data on Cl ions, some of the available data contain inconsistencies which need careful investigations. For example, recently, our extensive CI investigation [7] identified strong configuration mixing among some levels of Cl II and resolved, in agreement with a recent elaborate  $R$ -matrix calculation [8], the controversy regarding the lowest  $^1P^o$  level of Cl II. Also, incompatibilities between the the NIST database [9], based upon Martin's paper [10], and the Moore tables [11] exist on the Internet exist on the positions of several energy levels including the lowest  $^1P^o$  level. Having realized that there exists very little data on Cl V, we have studied various spectroscopic data of this ion by using the CIV3 program of Hibbert [12] and Glass and Hibbert [13].

## 2 Method of calculation

The wave function for each level of interest can be expressed as

$$\Psi_i(JM_J) = \sum_{j=1}^K b_{ij} \phi_j(\alpha_j L_j S_j JM_J), \quad (1)$$

where each of the  $K$  single-configuration functions  $\phi_j$  are constructed from one-electron functions and  $\alpha_j$  defines coupling of the orbital  $L_j$  and spin  $S_j$  angular momenta

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**Table 1.** Clementi-type orbitals and their expansion parameters in equation (2) for some optimized orbitals.

orbitals	$p_i$	$\xi_i$	$C_i$
3d	3	4.6240019	0.1208319
	3	2.0195494	0.9275762
4s	1	13.5514705	0.0738742
	2	6.7244806	0.3016754
	2	6.2600168	-0.5818683
	3	1.5137710	-1.8945209
	3	2.3799601	1.5541112
4p	2	1.1206691	2.2089533
	2	7.9106838	0.1171882
	3	2.3122787	-1.9249275
4d	3	2.4047973	0.5922326
	4	1.2179446	-1.0941039
4f	4	1.2955121	1.000

to give the total angular momentum  $J$ . The mixing coefficients  $b_{ij}$  are obtained by diagonalizing the Breit-Pauli Hamiltonian with respect to the basis  $\Psi_i$ . The radial part of the one-electron functions is expressed in analytic form as a sum of Slater-type orbitals,

$$P_{nl}(r) = \sum_{i=1}^k C_i [(2\xi_i)^{2p_i+1}/(2p_i)!]^{1/2} r^{p_i} \exp(-\xi_i r), \quad (2)$$

where  $n$  and  $l$ , respectively, are the principal and orbital quantum numbers and  $C_i$ ,  $\xi_i$  and  $p_i$  are expansion parameters. We started with Hartree-Fock 1s, 2s, 2p, 3s, and 3p orbitals from Clementi and Roetti [14]. Then the orbitals 3d, 4s, 4p, 4d and 4f in the form of equation (2) were optimized on the energies of the  $3s^2 3d(^2D)$ ,  $3s^2 4s(^2S)$ ,  $4s^2 4p(^2P^o)$ ,  $4s^2 4d(^2D)$  and  $4s^2 4f(^2F^o)$  levels, respectively using the CIV3 code [12,13]. The expansion parameters in equation (2) are determined variationally and using the orthogonality condition

$$\int_0^\infty P_{nl}(r)P_{n'l}(r)dr = \delta_{nn'}. \quad (3)$$

These parameters are presented Table 1.

In the present paper we are interested in the fine-structure levels belonging to the following basic configurations:  $3s^2 3p(^2P^o)$ ,  $3s3p^2(^2,^4P, ^2D, ^2S)$ ,  $3s^2 3d(^2D)$ ,  $3p^3(^4S^o, ^2P^o, ^2D^o)$ ,  $3s3p(^3P)3d(^2,^4P^o, ^2,^4D^o, ^2,^4F^o)$ ,  $3s3p(^1P)3d(^2P^o, ^2D^o, ^2F^o)$ ,  $3s^2 4s(^2S)$ ,  $3s^2 4p(^2P^o)$ ,  $3s^2 4d(^2D)$  and  $3s3p(^3P)4s(^2,^4P^o)$ . These configurations constitute 23 LS states and 49 fine-structure levels. In order to allow sufficient configuration mixing we have considered one-, two- and three-electron promotional configurations with respect to the ground configuration  $3s^2 3p(^2P^o)$ . This means that we began our LS energy calculation with such an extended set of configurations (upto three-electron promotions) and then drop those configurations whose eigenvector strengths are less than 0.001. Apart from the above basic configurations the following one-, two-, and three-electron promotional

configurations remained in the CI expansion. They are  $3s3p4d$ ,  $3s3p4s$ ,  $3s^2 4p$ ,  $3s^2 4f$ ,  $3p3d^2$ ,  $3p4s^2$ ,  $3p4f^2$ ,  $3p4d^2$ ,  $3p4p^2$ ,  $3s4s4p$ ,  $3s4p4d$ ,  $3s4d4f$ ,  $3p3d4s$ ,  $3p4s4d$ ,  $3p4p4f$ ,  $3p3d4d$ ,  $3p4d^2$ ,  $3s4s4f$ ,  $3s3d4f$ ,  $3d^2 4p$ ,  $3d^2 4f$ ,  $3d4s4f$ ,  $4s4p4d$ ,  $3d4d4f$ ,  $3d4p4d$ ,  $4p4d^2$ ,  $3d4s4p$ ,  $4d^2 4f$ ,  $4s^2 4f$ ,  $4p^2 4f$ ,  $4p^3$ ,  $4p4f^2$  for the odd parity states and  $3s3p4p$ ,  $3s^2 4d$ ,  $3s3p4f$ ,  $3s3d^2$ ,  $3s3d4d$ ,  $3p^2 3d$ ,  $3p^2 4s$ ,  $3p^2 4d$ ,  $3p3d4p$ ,  $3p3d4f$ ,  $3p4s4p$ ,  $3p4p4d$ ,  $3p4d4f$ ,  $3s3d4s$ ,  $3s4p4f$ ,  $3p4s4f$ ,  $3d^2 4s$ ,  $3d4s4d$ ,  $3d4p4f$ ,  $3d^2 4d$ , for the even parity states. It is important to note that among both the odd and even configurations, many are actually three-electron promotional configurations with one, two or (all) three electron(s) in the  $n = 4$  complex. This clearly advocates the need to account for the CI mixing between  $n = 3$  and  $n = 4$  levels. Our experience [7] in this regard indicates that configurations with some electrons in the  $n = 5$  complex might be worth including at least for the fine-structure levels towards the end of Table 2. However, this would drastically increase the size of the configurations and therefore avoided in the present calculation.

### 3 Result and discussions

In the present calculation our *ab initio* energies are adjusted slightly using a fine tuning technique [15] within the prescription of the CIV3 program. This technique is often very helpful to avoid many-electron promotional configurations while the calculated energies can be obtained close enough to the measured values. In the present case we have adjusted our *ab initio* energies to reproduce NIST values as close as possible. In Table 2 we compare our adjusted excitation energies with those obtained from NIST compilations, results of Fawcett [3] and those of Fischer [16]. In the last column of this table we present the leading percentage of the corresponding level in the ‘‘Index’’ column. Any number of the format  $M(N)$  following the leading percentage means that  $M\%$  of the level number  $N$  are contributing in terms of the configuration mixing. This means that whenever the leading percentage is close or equal to 100 the corresponding level is almost a pure state. In all other cases they are coupled with the next leading level  $N$ , by  $M\%$ .

From the Table 2 we observe that for the multiplets of  $^4P(J = 1/2, 3/2 \text{ and } 5/2)$  belonging to  $3s3p^2$  configuration which are almost pure levels, our results have the closest agreement with those of NIST while Fawcett’s [3] results are the next best. For the next seven even levels belonging to  $3s3p^2$  and  $3s^2 3d$  configurations, Fawcett’s [3] results compare more favourably with the NIST results than ours. All these seven levels have either strong or weak (not shown in the table) coupling with other levels. This is rather unexpected since coupling due to the configuration mixing is accounted for more comprehensively in the present calculation than in the Fawcett’s [3] calculation who considered configurations belonging to the  $n = 3$  complex only. Both methods include important relativistic effects. For the remaining levels in Table 2 our results agree better with the NIST recommended data than

**Table 2.** Comparisons of energy levels (in  $\text{cm}^{-1}$ ) for Cl V from experimental compilations of NIST data, present calculation and BCF and CFF represents earlier calculation of Fawcett [3] and Fischer [16] respectively. The numbers in the form  $M(N)$  mean the next leading composition is  $M\%$  of the level number  $N$  under the index column.

Index	Conf.	level	NIST	BCF	present	CFF	leading%
1	$3s^23p$	$^2P_{1/2}$	0.0		0.0		
2		$^3P_{3/2}$	1490.8		1483.1	1469.80	95
3	$3s3p^2$	$^4P_{1/2}$	86000	85005	86016.3	85610.48	99
4		$^4P_{3/2}$	86538	85542	86555.0	86140.97	99
5		$^4P_{5/2}$	87381	86392	87395.6	86974.89	99
6		$^2D_{3/2}$	113234	113248	112308.0	113868.0	80, 17(11)
7		$^2D_{5/2}$	113306	113291	112375.0	113942.6	80, 17(12)
8		$^2S_{1/2}$	146644	146647	146791.9	148449.9	96
9		$^2P_{1/2}$	157931	157928	158184.7	161136.8	94
10		$^2P_{3/2}$	158892	158902	159138.9	162092.3	94
11	$3s^23d$	$^2D_{3/2}$	185861	185858	187137.9	188393.2	78, 17(6)
12		$^2D_{5/2}$	185893	185895	187176.3	188419.4	78, 17(7)
13	$3p^3$	$^2D_{3/2}$	222650	225481	222018.0	221528.0	60, 21(31), 16(44)
14		$^2D_{5/2}$	222650	225635	222070.7	221665.6	60, 21(30), 16(45)
15		$^4S_{3/2}$	233757	232754	233790.0	234231.2	98
16	$3s3p(^3P)3d$	$^4F_{3/2}$		245203	247302.0	246235.8	100
17		$^4F_{5/2}$		245534	247569.9	246508.4	100
18		$^4F_{7/2}$		246003	247950.7	246930.9	100
19		$^4F_{9/2}$		246616	248451.2		100
20	$3p^3$	$^2P_{3/2}$	252930	256787	253584.9	253329.1	73, 16(38), 4(41)
21		$^2P_{1/2}$	252990	256854	253634.6	253281.2	73, 16(39), 4(40)
22	$3s^24s$	$^2S_{1/2}$	256313		256390.3	256742.2	95
23	$3s3p(^3P)3d$	$^4P_{5/2}$	269986	269000	270026.6	269390.1	97
24		$^4P_{3/2}$	270423	269418	270458.8	269826.7	97
25		$^4P_{1/2}$	270745	269727	270789.8	270138.6	98
26		$^4D_{1/2}$	272596	271548	272669.4	272381.8	98
27		$^4D_{3/2}$	272757	271729	272840.0	272527.6	96
28		$^4D_{5/2}$	272919	271923	272998.6	272686.1	97
29		$^4D_{7/2}$	273020	272075	273084.3	272802.5	99
30		$^2D_{5/2}$		281912	285177.7	282484.7	42, 17(45), 39(14)
31		$^2D_{3/2}$		281935	285239.0	282521.3	42, 17(44), 39(13)
32		$^2F_{5/2}$			300249.6	293899.6	64, 33(37)
33		$^2F_{7/2}$			301307.1	295086.5	63, 33(36)
34	$3s^24p$	$^2P_{1/2}$			305178.8	295324.9	94
35		$^2P_{3/2}$			305504.0	295756.3	94
36	$3s3p(^1P)3d$	$^2F_{7/2}$			329692.9	321267.1	55, 34(33), 7(51)
37		$^2F_{5/2}$			329970.7	321569.3	55, 34(32)
38	$3s3p(^3P)3d$	$^2P_{3/2}$		328334	330892	323752.5	79, 17(20)
39		$^2P_{1/2}$		326844	331269.1	324072.4	79, 16(21)
40	$3s3p(^1P)3d$	$^2P_{1/2}$		345977	346971.0	337807.5	84, 7(21), 2(49)
41		$^2P_{3/2}$		346281	347133.1	337880.9	84, 7(20)
42	$3s^24d$	$^2D_{3/2}$			349634.9		94
43		$^2D_{5/2}$	349511		349636.2		94
44	$3s3p(^1P)3d$	$^2D_{3/2}$	349511	345909	349850.7	338160.6	61, 34(31)
45		$^2D_{5/2}$		346273	350037.1	342228.0	61, 34(30)
46	$3s3p(^3P)4s$	$^4P_{1/2}$	353445		353499.2	352299.2	99
47		$^4P_{3/2}$	353978		354031.8	352791.8	99
48		$^4P_{5/2}$	354925		354977.3	353661.7	99
49		$^2P_{1/2}$			367212.6		94
50		$^2P_{3/2}$			368087.7		93

**Table 3.** Oscillator strengths and transition probabilities ( $s^{-1}$ ) for some dipole-allowed transitions in Cl V.  $f_L$  and  $A_L$  are the present oscillator strengths and transition probabilities in length form.  $f(BCF)$  are the oscillator strengths of Fawcett [3],  $A(CFF)$  are the transition probabilities of Fischer [16] and  $A(NIST)$  those of NIST.  $a(b) = a \times 10^b$ .

lower	level	upper	level	$f_L$	$f(BCF)$	$A_L$	$A(CFF)$	$A(NIST)$		
$3s^2 3p$	$^2P_{1/2}$	$3s^2 3d$	$^2D_{3/2}$	1.045	1.02	1.220(10)	1.253(10)			
		$3s^2 4s$	$^2S_{1/2}$	0.0808		3.544(09)	3.849(09)	4.00(09)		
	$^2P_{3/2}$	$3s^2 3d$	$^2D_{5/2}$	0.9421	0.917	1.490(10)	1.485(10)			
		$3s^2 4s$	$^2S_{1/2}$	0.0824		7.146(09)	7.797(09)	7.90(09)		
	$^2P_{1/2}$	$3s3p^2$	$^2P_{1/2}$	$^2P_{1/2}$	0.4329	0.445	7.367(09)	7.335(09)		
			$^2P_{3/2}$	$^2P_{3/2}$	0.2366	0.245	2.028(09)	2.133(09)		
	$3s3p^2$	$^4P_{1/2}$	$3p^3$ $3s3p(^3P)3d$	$^2D_{3/2}$	0.0472	0.060	1.985(08)	2.782(08)	2.30(09)	
				$^2P_{3/2}$	$^2P_{3/2}$	0.5711	0.572	9.468(09)	1.014(10)	
				$^2D_{5/2}$	$^2D_{5/2}$	0.0398	0.050	2.178(08)	3.053(08)	2.60(09)
				$^2D_{3/2}$	$^2D_{3/2}$	0.0036	0.0042	2.908(07)	4.140(07)	4.30(08)
$^4S_{3/2}$				$^4S_{3/2}$	0.2363	0.240	1.721(09)	1.746(09)		
$^4P_{3/2}$				$^4P_{3/2}$	0.4515	0.485	5.123(09)	5.209(09)		
$3s3p^2$	$^4P_{3/2}$	$3p^3$ $3s3p(^3P)3d$	$^4D_{1/2}$	0.4780	0.470	1.111(10)	1.126(10)			
			$^4D_{3/2}$	0.3857	0.355	4.490(09)	4.495(09)			
			$^4S_{3/2}$	0.2353	0.240	3.402(09)	3.449(09)			
			$^4P_{5/2}$	0.2794	0.307	4.182(09)	4.315(09)			
			$^4D_{3/2}$	0.3725	0.382	8.623(09)	8.717(09)			
			$^4D_{5/2}$	0.5499	0.527	8.501(09)	8.491(09)			
$3s3p^2$	$^4P_{5/2}$	$3p^3$ $3s3p(^3P)3d$	$^4S_{3/2}$	0.2340	0.238	5.018(09)	5.081(09)			
			$^4P_{5/2}$	0.1902	0.172	4.231(09)	4.216(09)			
			$^4D_{5/2}$	0.2588	0.277	5.947(09)	6.082(09)			
			$^4D_{7/2}$	0.8404	0.850	1.450(10)	1.466(10)			
			$^2D_{3/2}$	$^2D_{3/2}$	0.5629	0.552	1.123(10)	1.035(10)		
			$^2F_{5/2}$	$^2F_{5/2}$	0.3423	0.372	5.347(09)	5.047(09)		
$3s3p^2$	$^2D_{5/2}$	$3p^3$ $3s3p(^3P)3d$	$^2D_{5/2}$	0.5794	0.566	1.154(10)	1.062(10)			
			$^2S_{1/2}$	$^2P_{1/2}$	0.4975	0.435	1.129(10)	1.110(10)		
			$^2P_{1/2}$	$^2P_{1/2}$	0.2349	0.230	4.694(09)	3.283(09)		
			$^2P_{3/2}$	$^2D_{5/2}$	1.492	1.41	2.417(10)	2.102(10)		

the other two sets of results presented in this table. It is worth noting that the fine-tuning technique adopted in the present study improved the present *ab initio* energies by only about a percent.

The configuration mixing among many of the levels is found to be very strong. As an example the  $3p^3(^2D_{3/2})$ ,  $3s3p(^3P)3d(^2D_{3/2})$  and the  $3s3p(^1P)3d(^2D_{3/2})$  couples very strongly although energetically they are well separated. The strong coupling among these levels makes their identification quite difficult. A closer look at the last column of level numbers 30 and 31 shows that 42% of level 30 couples with 39% of level 14 and 42% of level 31 couples with 39% of level 13 — a difference of only 3%. Fortunately, levels 13 and 14 were clearly identified earlier with a significant difference in percentage composition.

In Table 3 we compare some of our oscillator strengths (length form only) with those of Fawcett [3] and transition probabilities with those of Fischer [16] and NIST for some dipole allowed transitions. It is found that the present oscillator strengths agree closely with those of Fawcett [3] and Fischer [16] (not shown in the table). Also for the transition amplitudes our results agree very well with those

of Fischer [16]. However, three of the five NIST transition amplitudes differ with the present as well as those of Fischer [16] by an order of magnitude. For the remaining two transitions the NIST data agree with the two calculations. It is interesting to note that the accuracy rating of the former three NIST values is very poor (E) *versus* reasonable accuracy (C) for the remaining two transitions. In Table 4 we compare present line strengths for some allowed transitions with those of Fischer [16]. The agreement between the two calculations are very good.

Finally in Table 5 we compare the present lifetimes for some relatively longer lived levels with those obtained by Fischer [16]. We note that the  $^4P_{3/2}$  level belonging to the first excited configuration  $3s3p^2$  have a very high life time of about 23.0 microseconds. Life time of  $3s3p(^3P)3d(^4F_{3/2,5/2,7/2})$  levels are nearly two orders of magnitude longer than life time of  $3p^3(^2D_{3/2,5/2})$  levels.

## 4 Conclusion

Forty-nine fine-structure levels of Cl V relative to the ground state  $3s^2 3p(^2P_{1/2})$  are calculated in the

**Table 4.** Comparison of line strength for some large transitions in Cl V. CFF represents the results of Fischer [16].

lower	level	upper	level	present	CFF
$3s^2 3p$	$^2P_{1/2}$	$3s3p^2$	$^2P_{1/2}$	1.802	1.825
		$3s^2 3d$	$^2D_{3/2}$	3.676	3.700
	$^2P_{3/2}$	$3s3p^2$	$^2P_{1/2}$	1.066	1.077
			$^2P_{3/2}$	4.770	4.829
$3s3p^2$	$^4P_{1/2}$	$3s^2 3d$	$^2D_{5/2}$	6.681	6.729
		$3p^3$	$^4S_{3/2}$	1.053	1.050
	$3s3p(^3P)3d$		$^4P_{3/2}$	1.612	1.645
			$^4D_{1/2}$	1.686	1.706
$3s3p^2$	$^4P_{3/2}$		$^4D_{3/2}$	1.359	1.359
		$3p^3$	$^4S_{3/2}$	2.105	2.097
	$3s3p(^3P)3d$		$^4P_{5/2}$	2.005	2.077
			$^4D_{3/2}$	2.633	2.658
		$^4D_{5/2}$	3.884	3.873	

**Table 5.** Life times (in seconds) for some relatively longer lived levels of Cl V. CFF represents the result of Fischer [16].  $a(-b) = a \times 10^{-b}$ .

level	present	CFF
$3s3p^2 ^4P_{1/2}$	4.460(-06)	3.987(-06)
$3s3p^2 ^4P_{3/2}$	2.298(-05)	2.146(-05)
$3s3p^2 ^4P_{5/2}$	9.944(-06)	8.050(-06)
$3s3p^2 ^2D_{3/2}$	4.393(-09)	3.129(-09)
$3s3p^2 ^2D_{5/2}$	4.591(-09)	3.276(-09)
$3p^3 ^2D_{3/2}$	1.931(-09)	2.064(-09)
$3p^3 ^2D_{5/2}$	1.916(-09)	2.041(-09)
$3s3p(^3P)3d ^4F_{3/2}$	4.944(-07)	3.825(-07)
$3s3p(^3P)3d ^4F_{5/2}$	4.151(-07)	3.047(-07)
$3s3p(^3P)3d ^4F_{7/2}$	4.855(-07)	3.429(-07)

intermediate coupling scheme which include relativistic effects such as spin-orbit, spin-spin, spin-other-orbit, mass correction and Darwin terms. Significant coupling are noted among the configurations belonging to  $n = 3$  and  $n = 4$  complexes. It is, therefore, concluded that both relativistic effects and a reasonably large size of interacting configurations are essential for an atomic data calculation of Cl V. Oscillator strengths, transition probabilities and

line strengths for some optically allowed transitions are also presented and are in good agreement with available data. Lifetimes of some excited levels are found to be of the order of microseconds.

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