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# Atomic data from the IRON Project.
# IX. Electron excitation of the $^2\mathbf{P}^\circ_{\frac{3}{2}} - {}^2\mathbf{P}^\circ_{\frac{1}{2}}$ fine-structure transition in chlorine-like ions, from Ar II to Ni XII

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**Abstract.** — Calculated effective collision strengths for the ground term fine-structure transitions of 11 chlorine-like ions (17 electrons) from Ar II to Ni XII are presented. There is currently very little published data for this sequence and so there is a strong motivation to satisfy the need for this information and to improve upon the accuracy of previous work where it does exist. The data are calculated using R-matrix techniques and are provided over a temperature range from $10^3$ K up to $10^7$ K over which the target models should be valid. Accuracy for the effective collision strengths is in the region of 10%. An independent calculation on Fex recently published by Mohan et al. (ApJ 434, 389) is shown to be wrong for this transition because of their omission of important low-energy contributions.

**Key words:** atomic data

## 1. Introduction

There is an increasing demand for electron excitation data from many fields ranging from laser design, fusion reactor research and industrial plasma generation through to astrophysics. Indeed, researchers in the latter area will require and insist upon reliable cross sectional information to enable and assist with the interpretation of data obtained from the Infrared Space Observatory (ISO) and the Solar and Heliospheric Observatory (SOHO) when they are operational.

The results presented here are part of a systematic endeavour by the IRON Project (Hummer et al. 1993, hereafter referred to as Paper I) to provide essential theoretical data for such needs. This paper forms a part of the first stage goal of the Project in obtaining effective collision strengths for fine-structure transitions for a range of astrophysically important ions, in this case the chlorine-like iso-electronic sequence from Ar II ($Z$=18) to Ni XII ($Z$=28). A full list of all the previous Iron Project papers are given in the references.

Pradhan & Gallagher (1992) list sources of theoretical electron excitation data published since the 1950's and demonstrate the scarcity of work on the chlorine sequence within the last twenty years (Blaha 1969; Krueger & Czyzak 1970). The exception to this are more recent examinations of the astrophysically significant ion Fe X (Mason 1975; Nussbaumer 1970) but the optically forbid-den fine-structure transitions have been largely neglected. Where data exists the accuracy may not be better than 30%. The current work hopes to fill the current void with data and improve upon the validity and accuracy of that earlier work.

The descriptions of the theory and computational aspects of this work are more fully described in Paper I, the parent IRON Project publication. An account of the particular details of the calculation are in the next section followed by a presentation of the results with comparisons with previous works.

## 2. Present calculations

The scattering calculations were carried out using the R-matrix method in LS coupling; collision strengths for the fine-structure transitions were obtained using an algebraic transformation to intermediate coupling, as described in Sect. 2.6 of Paper I. All terms arising from the $3s^2 3p^5$, $3s 3p^6$ and $3s^2 3p^4 3d$ configurations were included explicitly in the expansion of the total wavefunction; a total of 14 terms.

The target wavefunctions were generated using the CIV3 program (Hibbert 1975) in conjunction with the radial functions calculated by Clementi & Roetti (1974). The latter provide the 1s,2s,2p,3s and 3p orbitals. The exponents for the 3d orbital (Table 1) which were required for the target states were obtained by optimisation, i.e. by

**Table 1.** Optimised exponents for the 3d orbital

| Z | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 |
|---|----|----|----|----|----|----|----|----|----|----|----|
|  | 3.21429 | 4.22506 | 4.87578 | 5.47824 | 6.20608 | 6.82341 | 7.38334 | 8.01472 | 8.30174 | 9.13301 | 9.74224 |
|  | 1.36666 | 1.88454 | 2.29026 | 2.67025 | 3.06279 | 3.43164 | 3.78911 | 4.15033 | 4.46250 | 4.84879 | 5.20660 |

the normal method of minimising the energy of the corresponding wavefunction. The following configurations were subsequently used in the expansion of the target wavefunction; $3s3p^53d$, $3s^23p^33d^2$, $3s^23p^43d$, $3s3p^43d^2$. The derived energies of the $3s^23p^5$ to $3s3p^6$ transition were in good agreement with observed data (Table 2) and were not subsequently revised.

**Table 2.** Target data. Target $^2P^\circ - ^2S$ term separations from this work ($E_{IP}$) together with observed separations ($E_{obs}$) and fine-structure splitting $E_{fs}$ (both taken from Fawcett 1987, Table VI) are given in Rydbergs. The length and velocity forms of the calculated oscillator strengths ($f_l$,$f_v$) are compared to the oscillator strengths ($f$) also by Fawcett (1987)

| Z | $E_{IP}$ | $E_{obs}$ | $E_{fs}$ | $f_l$ | $f_v$ | $f$ |
|---|---------|----------|---------|-------|-------|-----|
| 18 | 0.9899 | 0.9777 | 0.013 | 0.011 | 0.006 | 0.004 |
| 19 | 1.1799 | 1.1705 | 0.020 | 0.021 | 0.015 | 0.008 |
| 20 | 1.3677 | 1.3607 | 0.028 | 0.027 | 0.021 | 0.015 |
| 21 | 1.5549 | 1.5499 | 0.039 | 0.031 | 0.024 | 0.022 |
| 22 | 1.7416 | 1.7387 | 0.053 | 0.033 | 0.026 | 0.028 |
| 23 | 1.9282 | 1.9273 | 0.070 | 0.034 | 0.028 | 0.032 |
| 24 | 2.1146 | 2.1157 | 0.090 | 0.034 | 0.028 | 0.035 |
| 25 | 2.3007 | 2.3042 | 0.114 | 0.034 | 0.029 | 0.036 |
| 26 | 2.4870 | 2.4929 | 0.143 | 0.034 | 0.028 | 0.037 |
| 27 | 2.6726 | ... | 0.177 | 0.034 | 0.028 | ... |
| 28 | 2.8778 | 2.8704 | 0.215 | 0.037 | 0.030 | 0.039 |

Fawcett (1987) calculated energy levels for the optically allowed 3-3 transitions of the the chlorine-like sequence (from $Z=18$ to 28, except $Z=27$) using Slater parameter optimisation in conjunction with the Hartree-Fock-Relativistic (HFR) and Multiconfiguration-Dirac-Fock (MCDF) methods. In that work the ab initio calculations were adjusted to bring the resulting energies in line (circa 0.1%) with observed data. It was noted that both HFR and MCDF methods yielded almost identical energies (differing insignificantly) but that the requirement of tuning to match observed data was necessary for complete accuracy. The ab initio energies we show in this paper are within 1% of those observed (and hence the HFR and MCDF calculations also).

For all the ions in the sequence the 4s term lies above the 3d level, except for Ar II which suggests that configuration mixing between those two terms for that ion is important. Fawcett (1987) performed a study on the configuration mixing showing that the $3s^23p^44s$ term does couple very strongly with the $3s^23p^43d$ for the first few ions, namely Ar II, K III and Ca IV. Including the 4s term would substantially increase the complexity of the calcula-

tion; however, a test calculation was performed for Ca IV which showed little significant contribution from the 4s term.

## 3. Results

The *effective collision strength* ($\Upsilon$) is obtained by integrating the collision strength ($\Omega$) over a Maxwellian distribution of electron velocities for a given temperature ($T$). The $\log T$ range chosen for each ion was $-1.2$ to $+0.8$ dex of the temperature of maximum ionic abundance given by Shull and Van Steenberg (1982). The results are tabulated in Table 3.

**Table 3.** Effective collision strengths $\Upsilon(^2P^\circ_{\frac{3}{2}} - ^2P^\circ_{\frac{1}{2}})$ for chlorine-like ions. The temperature range ($K$) is restricted to within regions where the data is considered reliable

| $\log T$ | $Z=18$ | $Z=19$ | $Z=20$ | $Z=21$ | $Z=22$ |
|---------|--------|--------|--------|--------|--------|
| 3.20 | 2.48 | ... | ... | ... | ... |
| 3.40 | 2.54 | ... | ... | ... | ... |
| 3.60 | 2.63 | 2.22 | ... | ... | ... |
| 3.80 | 2.77 | 2.21 | ... | ... | ... |
| 4.00 | 2.93 | 2.21 | 1.00 | ... | ... |
| 4.20 | 3.09 | 2.20 | 1.12 | 6.35 | ... |
| 4.40 | 3.19 | 2.19 | 1.35 | 6.00 | 3.48 |
| 4.60 | 3.20 | 2.21 | 1.77 | 5.49 | 3.56 |
| 4.80 | 3.13 | 2.30 | 2.39 | 4.95 | 3.46 |
| 5.00 | 2.97 | 2.39 | 2.80 | 4.39 | 3.22 |
| 5.20 | 2.71 | 2.36 | 2.98 | 3.77 | 2.88 |
| 5.40 | ... | 2.17 | 2.82 | 3.07 | 2.46 |
| 5.60 | ... | 1.86 | 2.43 | 2.41 | 2.01 |
| 5.80 | ... | ... | 1.97 | 1.84 | 1.58 |
| 6.00 | ... | ... | 1.53 | 1.39 | 1.22 |
| 6.20 | ... | ... | ... | 1.07 | 0.94 |
| 6.40 | ... | ... | ... | ... | 0.73 |
| $\log T$ | $Z=23$ | $Z=24$ | $Z=25$ | $Z=26$ | $Z=27$ | $Z=28$ |
| 4.60 | 2.39 | ... | ... | ... | ... | ... |
| 4.80 | 2.27 | 1.76 | 2.48 | ... | ... | ... |
| 5.00 | 2.15 | 1.93 | 2.58 | 3.38 | 1.36 | 1.68 |
| 5.20 | 2.00 | 2.00 | 2.50 | 3.15 | 1.25 | 1.67 |
| 5.40 | 1.78 | 1.87 | 2.24 | 2.97 | 1.08 | 1.51 |
| 5.60 | 1.50 | 1.59 | 1.87 | 2.69 | 0.91 | 1.26 |
| 5.80 | 1.18 | 1.25 | 1.48 | 2.27 | 0.74 | 0.99 |
| 6.00 | 0.87 | 0.94 | 1.13 | 1.79 | 0.58 | 0.76 |
| 6.20 | 0.62 | 0.66 | 0.85 | 1.35 | 0.44 | 0.58 |
| 6.40 | 0.42 | 0.45 | 0.64 | 0.99 | 0.32 | 0.44 |
| 6.60 | 0.54 | 0.30 | 0.49 | 0.73 | 0.22 | 0.34 |
| 6.80 | 0.46 | 0.42 | 0.39 | 0.54 | 0.16 | 0.28 |
| 7.00 | ... | ... | ... | 0.40 | 0.23 | 0.23 |

A number of test calculations were performed, particularly for Ca IV, in order to establish the accuracy of the approximations made in this paper. Figure 1 shows the effective collision strength for Ca IV using 2, 14 and 18 term

**Table 4.** Comparison of collision strengths $\Omega(^2P^o_{\frac{3}{2}} - {}^2P^o_{\frac{1}{2}})$ with published data. Energies ($\epsilon$) are in Rydbergs scaled by the square of the charge on the ion ($E/z^2$). $\Omega_b$ are from Blaha 1969, $\Omega_k$ from Krueger & Czyzak 1970, $\Omega_{hm}$ from Mason 1975 and $\Omega_{ip}$ from present work

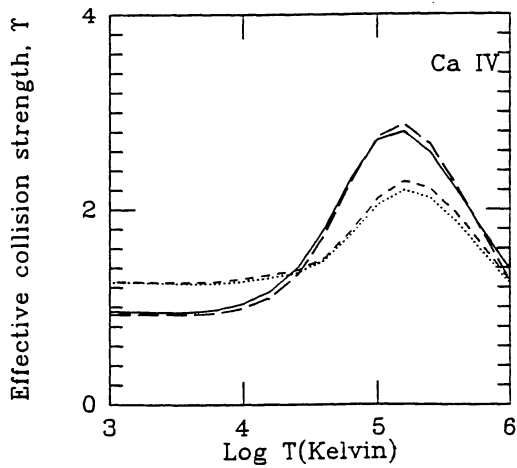| $\epsilon$ | $Z$ | $\Omega_b$ | $\Omega_k$ | $\Omega_{ip}$ | $\epsilon$ | $\Omega_k$ | $\Omega_{ip}$ | $\epsilon$ | $\Omega_k$ | $\Omega_{ip}$ | $\epsilon$ | $\Omega_{hm}$ | $\Omega_{ip}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.00 | | | | | 0.05 | | | 0.10 | | | 0.068 | | |
| | 18 | 1.353 | 0.635 | 2.33 | | 0.740 | 2.93 | | 0.857 | 3.36 | | | |
| | 19 | 1.191 | 1.776 | 2.21 | | 1.758 | 2.01 | | 1.640 | 1.95 | | | |
| | 20 | 1.153 | 1.056 | 0.95 | | 0.857 | 4.51 | | 0.746 | 6.95 | | | |
| | 21 | 0.940 | ... | 6.45 | | ... | | | ... | | | | |
| | 22 | 0.776 | ... | 10.58 | | ... | | | ... | | | | |
| | 23 | ... | 0.424 | 0.97 | | 0.387 | 0.83 | | 0.362 | 0.77 | | | |
| | 24 | ... | 0.370 | 0.65 | | 0.349 | 0.67 | | 0.308 | 0.34 | | | |
| | 25 | ... | 0.321 | 0.40 | | 0.287 | 1.21 | | 0.257 | 0.27 | | | |
| | 26 | 0.317 | 0.286 | 0.36 | | 0.245 | 0.60 | | 0.217 | 0.24 | | 0.27 | 0.25 |
| | 27 | 0.247 | 0.219 | 0.44 | | 0.211 | 0.43 | | 0.186 | 0.21 | | | |
| | 28 | ... | 0.250 | 4.88 | | 0.183 | 0.23 | | 0.161 | 0.19 | | | |



**Fig. 1.** Effective collision strength ($\Upsilon$) for the ion Ca IV. Dotted line: Breit-Pauli (2-term), Short-Dashed line: JAJOM (2-term), Continuous line: JAJOM (14-term [inc. 3d]), Long-Dashed line: JAJOM (18-term [inc. 4s])

models (labelled 'JAJOM"). The 2 term model includes just the $3s^23p^5$ and $3s3p^6$ terms, but with a 3d orbital introduced for correlation; the 14 term model is the one used for the whole iso-electronic sequence and includes the $3s^23p^43d$ terms; the 18 term model also includes $3s^23p^44s$ terms.

It is clear that the 3d terms affect the low-energy background as well as introducing further resonance effects, so the effective collision strength is reduced at low temperatures and enhanced at high temperatures. The inclusion of the 4s terms do not appear to have further significant effects; therefore it is concluded that the target state expansion has probably converged in this temperature range.

A further test calculation was performed for the 2-term model; this was a Breit-Pauli calculation, in which relativistic effects are introduced into the scattering Hamiltonian, as discussed in Paper I, and thus fine-structure effects are included ab initio. However, Fig. 1 shows that

for Ca IV, this does not make a significant difference from the algebraic recoupling model actually used in this paper.

## 4. Previous work

In Table 4 we compare the $^2P^o_{\frac{3}{2}-\frac{1}{2}}$ collision strength with the results of Blaha (1969), who used a weak coupling approximation with exchange and with Krueger & Czyzak (1970), who used a distorted wave approximation. It is clear from the present work that this will be affected by the presence of near-threshold resonances, which were not included in the earlier work. At higher energies for the more ionized ions these are not relevant and so the results are similar to within a few percent. Also shown in Table 4 is the result of Mason (1975) who used a distorted wave approximation with algebraic recoupling. Although the single energy at which she tabulated the collision strength lies closes to a resonance in our work, the agreement is good as expected.

**Table 5.** Comparison of effective collision strengths $\Upsilon(^2P^o_{\frac{3}{2}} - {}^2P^o_{\frac{1}{2}})$ with published data. $\Upsilon_n$ are from Nussbaumer (1970), $\Upsilon_{hm}$ from Mason (1975) and $\Upsilon_{ip}$ from present work. Temperature ($T$) is in log $K$

| $Z$ | $T$ | $\Upsilon_n$ | $\Upsilon_{hm}$ | $\Upsilon_{ip}$ |
|---|---|---|---|---|
| 26 | | | | |
| | 5.8 | 1.84 | 1.68 | 2.27 |
| | 6.0 | 2.55 | 1.68 | 1.79 |
| | 6.2 | 3.19 | 1.68 | 1.35 |
| | 6.4 | 3.68 | 1.68 | 0.99 |

In Table 5 we compare the effective collision strengths for Fe X, the only Cl-like ion for which several previous calculations have been performed. Both Mason (1975) and Nussbaumer (1970) calculated the effective collision strengths by only allowing for direct excitation to $^2P_{\frac{1}{2}}$ and radiative decay to that level from a few higher (ex-

cited) terms, and assuming that the collision strengths were constant with energy. Mason's $\Upsilon$ was also constant with temperature. We would not expect such unrealistic models to match present work but they are nonetheless included for the sake of completion. However our work shows the importance of resonances, i.e. the strong energy dependence of collision strength, and the need to obtain collision strengths accurately at low energies in order to calculate $\Upsilon$ reliably.

## 5. Conclusion

The effective collision strengths have been calculated for 11 chlorine-like ions from Ar II to Ni XII. This will help redress the present scarcity of data in this field. Although some data where already extant doesn't compare favourably with that presented here this can be explained by the more simplified models used in earlier works. It is concluded from the tests and comparisons made in Sect. 3 that, apart from Ar II, the results given in Table 3 should have an accuracy better than 10%.

After our paper was submitted, an independent calculation using similar techniques to ours was published by Mohan et al. (??). However, it is clear from their paper that they did not calculate collision strengths at energies below the first excited state, thus omitting all contributions to the $\Upsilon$ from this important resonance region. This leads to an underestimate in $\Upsilon \left( ^2P^o_{\frac{3}{2}} - ^2P^o_{1} \right)$ by a factor of 2 to 6, depending on the temperature and we have verified this effect by simulating their fault with our own data. We thus conclude that their data for that particular transition is wrong.

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