The Si ii intercombination multiplet in late-type stars

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SUMMARY
New atomic data are used to calculate the relative intensities of transitions within the Si ii 3s\(^2\) 3p\(^2\) \(P\)-3s3p\(^2\) 4\(P\) intercombination multiplet for plasma parameters appropriate to late-type stellar atmospheres. These ratios are found to be significantly different from those of Dufton & Kingston, principally due to changes in the radiative rates. A comparison with line ratios for the Sun (from Skylab S082B spectra) and late-type stars (from IUE data) indicates that although the new theoretical line ratios are in better agreement with observation, significant discrepancies still exist. Possible explanations for these discrepancies are briefly discussed.

1 INTRODUCTION
Resonance lines of Si ii are prominent features in the ultraviolet spectra of both the Sun (Doschek et al. 1976) and other late-type stars (see for example Judge 1986). Transitions within the 3s\(^2\)3p\(^2\)\(P\)-3s3p\(^2\) 4\(P\) multiplet at approximately 2340 Å, although weaker, are also well observed (Feldman et al. 1976). The relative strengths of these intercombination lines are potentially useful density diagnostics for the chromosphere and transition regions of late-type stars because the populations of the 3s3p\(^2\) 4\(P\) levels move from coronal to Boltzmann statistics for electron densities between approximately 10\(^8\) and 10\(^11\) cm\(^{-3}\) (Dufton & Kingston 1985). Unfortunately observed and theoretical line ratios for late-type stars (Judge 1986; Jordan & Judge 1988) are in poor agreement. In several cases the observed line ratios lie well outside the theoretical range and in particular beyond the high-density (i.e. Boltzmann statistics) limit. This theoretical limit is independent of the electron collision rates but does depend on the radiative rates. Hence if the discrepancy is due to uncertainties in the adopted atomic data, it is the radiative rates which are in error.

Here we present new estimates of the radiative rates deduced from sophisticated configuration interaction wavefunctions. Significant changes are found from the values deduced by Nussbaumer (1977), which have normally been adopted in previous studies. Our radiative rates are combined with improved electron impact collisional rates (Dufton & Kingston 1991) to calculate theoretical line intensity ratios for the Si ii intercombination multiplet. These are compared with observed values for the Sun and for late-type stars, and possible explanations of the discrepancies discussed.

2 ATOMIC DATA
2.1 Spontaneous radiative rates
The intercombination lines are allowed E1 lines due to the spin–orbit mixing of 3s3p\(^2\)\(P\)-3s3p\(^2\) 4\(P\) with the corresponding doublets. The mixing coefficients in the wavefunction and hence the corresponding radiative rates depend on the accuracy to which both the spin–orbit interaction and the multiplet energy splittings are calculated.

We have estimated transition probabilities for these intercombination lines using configuration interaction wavefunctions generated by the code civs (Hibbert 1975; Glass & Hibbert 1978). In our recent study of radiative rates for the Si ii 3s\(^2\)3p\(^2\)\(P\)-3s3p\(^2\) 4\(D\) multiplet at 1814 Å (Dufton et al. 1991), we considered an extensive configuration set that not only allowed for electron correlation amongst the valence electrons but also included core–valence interactions. Although these latter effects were small, they made a significant contribution to the very strong mixing between the 3s3p\(^2\)D and 3s\(^2\)d\(^2\)D states. However, for the 3s3p\(^2\) 4\(P\) \(J=\frac{5}{2}\) or \(J=\frac{3}{2}\) wavefunctions, core–valence interaction is less important as the cancellation due to the configuration mixing for the intercombination multiplet is not so severe. Hence here, we have limited the configuration set to those describing valence–shell correlation (see Dufton et al. 1991 for more details) and with these have constructed wavefunctions for all the relevant states. The fine structure was represented by the operator

\[
\sum_i \frac{K_i}{r_i^6} \cdot s_i,
\]
with \( s_i \) and \( I_i \) being the spin and orbital angular momentum of the \( i \)th electron. A reasonably good representation of the fine-structure mixing of the various states could be obtained with \( \xi_2 = 0.933Z \), \( \xi_3 = 1.0Z \) and with all other \( \xi_i \) taken to be zero.

Our calculated energy levels are shown in Table 1 where they are compared with experiment and the earlier calculations of Nussbaumer (1977). The present fine-structure splittings and the multiplet positions are in better agreement with experiment than are the earlier results of Nussbaumer, probably due to the more extensive set of configurations considered here. In calculating the transition probabilities listed in Table 2, we have made small adjustments to the diagonal elements of the Hamiltonian matrix, so that the calculated eigenvalue differences coincide with the corresponding experimental energy separations. This fine-tuning of calculations is particularly effective in improving transition probabilities of intercombination lines (see Hibbert 1979; Ojha, Keenan & Hibbert 1988). Our transition probabilities are generally larger than those of Nussbaumer, probably due to his use of calculated energy differences, which will lead to both the transition and the fine-structure energy differences being underestimated.

2.2 Electron impact collision rates

Electron impact excitation rates were taken from Dufton & Kingston (1991) and are based on the calculation of Kingston et al. (1983). They differ from those used by Dufton & Kingston (1985) in that they allow more carefully for the contribution of higher partial waves and for the effect of pseudo-resonances due to the inclusion of correlation orbitals in the bound state wavefunctions. However, for the transitions of importance in calculating the intercombination line strengths, the rates adopted here are not significantly different from those used by Dufton & Kingston (1985).

3 THEORETICAL LINE RATIOS

Si ii emission line ratios were calculated for lines within the intercombination multiplet using the same model ion and assumptions as discussed by Dufton & Kingston (1985). Briefly, the model ion consisted of the seven lowest levels of Si ii, with only electron impact and spontaneous radiative rates being considered. Additionally all transitions were considered to be optically thin, while transitions between ionization stages were assumed to be negligible compared with those within a given ionization stage. Further details and justification for these simplifications can be found in Dufton & Kingston.

Level populations and relative line strengths were calculated for a range of electron densities and temperatures. As discussed by Dufton & Kingston (1985), line ratios for transitions within the intercombination multiplet are not particularly sensitive to the adopted electron temperature, especially for electron densities greater than \( 10^6 \text{ cm}^{-3} \). Hence in Figs 1 and 2, we plot two line ratios for a representative electron temperature of \( 10^4 \text{ K} \) (Arnaud & Rothenflug 1985), viz.,

\[
R_1 = \frac{I(0.5-0.5) + I(1.5-2.5)}{I(1.5-0.5)} = \frac{I(2334.6) + I(2334.4)}{I(2350.2)}
\]

and

\[
R_2 = \frac{I(1.5-1.5)}{I(1.5-0.5)} = \frac{I(2344.2)}{I(2350.2)}
\]

where \( I(J-J') \) and \( I(x) \) are the intensities for a \( 3s^23p^2P_J-3s3p^4P_J \) transition and a line at a wavelength of \( x \AA \) respectively. In both cases, two curves are shown based on the radiative rates of Nussbaumer (1977) and our calculations discussed in Section 2.1; the former are effectively identical to those given by Dufton & Kingston (1985).
4 OBSERVATIONAL DATA

4.1 Solar data

The solar $R_1$ ratio for Si II has been deduced from S082B Skylab spectra by Dufton & Kingston (1985).

4.2 Late-type stars

$\textit{IUE}$ high resolution LWR spectra have been used previously to derive line intensity ratios for the Si II intercombination multiplet for late-type stars (see for example Judge 1986). Rather than use these previous measurements, we have preferred to consistently re-extract the spectra for these and other stars. The $\textit{IUE}$ catalogue for exposures taken before 1988 March 1 was searched for suitable LWR high-resolution images of stars with spectral types later than K0. Approximately 21 images were identified as potentially suitable but after reduction only 17 were found to yield reasonably exposed spectra in the region of the Si II multiplet, together with no significant evidence of large variability in line strengths between images exposed at different times.

In Table 3, we list the images, which were finally used to determine line strengths, together with the stellar spectral types (Hoffleit 1982).

The Si II multiplet is observed on orders 98 and 99 of the LWR image. These orders were extracted using the $\textit{iuedr}$ program (Rees & Giddings 1989) on the STARLINK computer network (Bromage 1984). Since these methods have become fairly standard we will describe them only in outline here. First, scans perpendicular to the dispersion direction were made and used to locate the position of the relevant spectral orders on the camera faceplate. These were used as input for the tracking algorithm within $\textit{iuedr}$. The resulting spectra were then put on an absolute flux scale using $\textit{iuedr}$ standard calibrations. As the Si II multiplet covers only a small wavelength range, the line intensity ratios are hardly affected by the calibration adopted.

Subsequent data analysis and in particular the calculation of total line fluxes were undertaken with the Emission Line Fitting (ELF) subroutines within the $\textit{dipso}$ program (Howarth & Murray 1988). Intensities were estimated by fitting the spectra with a number of Gaussian emission profiles and a slowly varying continuum. Since the Si II features at 2334 and 2350 Å were deemed unblended (see Section 5.2) they were fitted as follows. Initially, the positions (but not the relative separation for the two components in the 22334 Å feature) and the widths of the Gaussians were allowed to vary and a least-squares fit was made. The widths of the Gaussians were then fixed to the average and a final least-squares fit undertaken.

In Table 3, we tabulate the observed Si II ratio $R_1$ defined in Section 3 together with an estimate of its accuracy. This was categorized as follows:

(a) the most secure measurements with no serious background problems – random errors should be less than 20 per cent;
(b) reasonable measurements with random errors which are generally less than 50 per cent;
(c) uncertain measurements.

Note that the Si II lines at 2344.10 Å are severely blended with nearby Fe II lines, especially with those at 2344.28 Å. Hence although we have deduced values for the $R_2$ ratio in some of our targets, we do not believe that these are sufficiently reliable to tabulate in Table 3.
5 DISCUSSION

A comparison of the observed ratios, $R_1$, in Table 3 with the predicted values in Fig. 1 shows the agreement is better for the theoretical ratios based on our new radiative rates rather than those based on the rates of Nussbaumer (1977). However, the observed values still appear to be systematically smaller than those predicted. For example, 10 (out of 17) stellar ratios are more than 20 per cent below the theoretical high-density limit using our radiative rates, compared with 14 for the limit deduced from the rates of Nussbaumer. In some cases, this may be due to uncertainties in the observations but for certain images (e.g. $\alpha$ Tra LWP3736, LWP7612; $\epsilon$ Sco LWP3761) the discrepancies are larger than the estimated observational errors.

There are at least two possible explanations for this systematic difference, viz., errors in the atomic data or the observed ratios are unreliable, possibly due to blending. We consider these possibilities below.

5.1 Reliability of the atomic data

Although there may be errors in the collision rates (see Dufton & Kingston 1991 for a discussion of these), we consider here only the possibility of errors in the radiative rates. This is because it is these data that define the minimum value of the theoretical ratio when it is in its high-density limit. The emission feature at 2334 Å is a blend of two components. The shorter wavelength component arises from the same upper level $(3s3p^2P_1^2-3s3p^2P_3^0)$ as that for the line at 2350 Å. Hence the ratio of these two transitions will be independent of the plasma parameters (assuming the plasma is optically thin as should be the case for these spin forbidden transitions) and will be given by the branching ratio of approximately 1.3. This ratio is not particularly sensitive to the detail of the atomic physics calculation; for example Nussbaumer (1977) found a ratio of approximately 1.5 although the absolute rates differ by approximately 40 per cent. Hence this will define a reliable theoretical lower limit for $R_1$, assuming that the other Si $\Pi$ component in the 2334 Å blend has a negligible intensity. Such a ratio would have to be consistent with the observed ratios (and estimated errors) given in Table 3, although three ratios would still lie outside the range of the theoretical values.

Additionally the feature observed at 2334 Å is broader than the line at 2350.2 Å, indicating that the intensity of the longer wavelength component $(3s3p^2P_3^0-3s3p^2P_1^2)$ is significant and hence the theoretical limit deduced above it too low. This is confirmed by the radiative rates given in Table 2, which imply that the two components should have comparable strengths.

The radiative rate for this longer wavelength component mainly arises from mixing of the $3s3p^2P_1^2$ state with the $3s3p^2D_2$ and the $3s3p^2D_3$ states. Hence at first sight the difficulty in estimating the radiative rate for the $3s3p^2P_1^2-3s3p^2D_2$ transition (see Dufton et al. 1991 for details) might also affect the intercombination transition. However, a more careful investigation of the mixing coefficients indicates that in this case the cancellation is not so severe and hence the radiative rate for the $3s3p^2P_1^2-3s3p^2P_3^0$ transition should be secure. Hence we conclude that errors in the atomic data are unlikely to completely explain the difference between the theoretical and observed ratios of $R_1$.

5.2 Observational uncertainties

It seems improbable that the source of the discrepancy could be in the observations or their analysis. Although the signal-to-noise of the individual spectra varies considerably, the best spectra are well exposed with resulting uncertainties in line flux of typically 5 per cent. The possibility of blends cannot be entirely ruled out, but it should be noted that, given the sense of the discrepancy between theory and observation, it would have to be the $\lambda 2350.17$ Å line which is blended to resolve the problem. Furthermore, the discrepancy between theory and observation is, in the worst cases, about a factor of 3-4, requiring the proposed blending component to be stronger than the Si $\Pi$ line. The absorption at 2350 Å is consistently narrower than nearby allowed lines of, for instance, Fe $\Pi$ of comparable intensity (e.g. $\lambda 2362.02$ Å) by about 50 per cent, which implies that the proposed blend is unlikely to be an allowed transition. This is supported by the lack of correlation between the degree of discrepancy between theory and observation and the relative strength of the $\lambda 2350$ Å feature with respect to the nearby allowed lines.

As discussed in Section 4.2, we have also measured the ratio of the fluxes in the feature at 2344.2 Å to that at 2350.2 Å; the former is a blend of Fe $\Pi$ $\lambda 2344.3$ Å and Si $\Pi$ $\lambda 2344.1$ Å. Although these ratios provide upper limits to the ratio $R_2$ (defined in Section 3), they are generally close to, or below, our theoretical high-density limit of 0.7. For example the ratios for LWP3736 and LWP7612 ($\alpha$ Tra) are 0.39 and 0.41, respectively. This would again suggest that it is the $\lambda 2350.2$ Å component which is the source of the discrepancy.

We therefore conclude that although there is better agreement between observation and theory using the new radiative rates presented here, significant discrepancies still remain. Currently the source of these discrepancies remains unclear.

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