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THEORETICAL ELECTRON DENSITY AND TEMPERATURE SENSITIVE EMISSION LINE RATIOS FOR HELIUM-LIKE Si XIII COMPARED TO DITE TOKAMAK OBSERVATIONS

F.P. KEENAN, R. BARNESLEY*, J. DUNN*, K.D. EVANS*, S.M. McCANN and N.J. PEACOCK**

Department of Pure and Applied Physics, Queen's University of Belfast, Belfast BT7 1NN, IR-Northern, Ireland
*Department of Physics, University of Leicester, LE1 7RH, GB-Leicester, Great-Britain
**Culham Laboratory (EURATOM/UKAEA Fusion Association), OX14 3DB, GB-Oxford, Great-Britain

Abstract: New calculations of the electron density sensitive emission line ratio R (= f/i) and temperature sensitive ratio G (= (f+i)/r) in helium-like Si XIII are presented, where f, i and r are the forbidden 1s^2 1S - 1s2s 3S, intercombination 1s^2 1S - 1s2p 3P_{1,2} and resonance 1s^2 1S - 1s2p 1P transitions, respectively. A comparison of these with R and G ratios measured from x-ray spectra of the DITE tokamak, for which the electron density and temperature have been well determined, reveals excellent agreement between theory and observation, with discrepancies of typically less than 10%. This provides experimental support for the accuracy of the atomic data adopted in the line ratio calculations. The theoretical results may therefore be applied with confidence to the analysis of remote sources for which no independant electron density and temperature estimates exist, such as solar flares.

1. Introduction

Emission lines arising from transitions between the 1s^2 1S ground state and the 1s2l levels in helium-like ions are frequently observed in the x-ray spectra of high temperature laboratory plasmas, as well as the solar corona [1,2]. They may be used to infer the electron density and temperature of the emitting region through the well known line ratios R (= f/i) and G (= (f+i)/r) respectively, where f is the forbidden 1s^2 1S - 1s2s 3S transition, i the intercombination 1s^2 1S - 1s2p 3P_{1,2} lines and r the resonance 1s^2 1S - 1s2p 1P transition [3,4]. However to determine reliable theoretical ratios, accurate atomic physics data must be employed, especially for electron excitation rates and f-values [3].

Over the past few years several authors have calculated electron impact excitation rates for He-like ions. Probably the most accurate currently available are those for C V, O VII and Mg XI derived with the R-matrix code [5] by Tayal and Kingston [6-9], and the results for Ca XIX and Fe XXV estimated by Pradhan [10] in the distorted wave approximation [11]. Keenan and co-workers [12-17] have shown that the theoretical R and G ratios determined using either the above atomic data or excitation rates for other He-sequence members interpolated from these [18] are in much better agreement with solar active region and flare observations than are previous calculations [19].

For He-like ions with atomic numbers Z > 12, the R ratio is in its low density limit for values of N_e (\leq 10^{12} \text{ cm}^{-3}) typically found under solar conditions [19]. However this is not the case with tokamak laboratory plasmas, where the densities may be several orders of magnitude larger [20], and hence R in high Z species should be useful as an electron density diagnostic. In this paper we use the Keenan et al [18] excitation rate calculations for Si XIII to derive R and G ratios for this ion, and compare these with observational data from the DITE tokamak.

2. Atomic data

The model ion for Si XIII was similar to those adopted for other He-like ions by Keenan and his co-workers [12-17]. Briefly, the 23 1s^nl states with n < 6 and l < 3 were included in the calculations, making a total of 37 levels when the fine structure splitting in the 3P and 3D terms was included. Energies of these levels were taken from Martin and Zalubas [21].

Electron impact excitation rates from the 1s^2 1S ground state to the n = 2 and 3 levels were obtained from Keenan et al [18], while for those among n = 2 the results of Pradhan et al [22] and
Zhang and Sampson [23] were adopted. Rates to or between higher lsnl states were either estimated from the above using the $n^{-3}$ scaling law [24] or taken from Sampson et al [25].

Einstein A-coefficients for transitions from the $n = 2$ levels were obtained from Lin et al [26], the results of Lin et al [27] and Cohen and McEachran [28] being used for $n > 2$. As noted by, for example, Pradhan [29], inner-shell ionisation of the Li-like ion and dielectronic and radiative recombination of the R-like ion are important mechanisms in determining the level populations of the relevant He-like ion. We have included these processes in the present analysis by employing the rate coefficients of Mewe and Schrijver [30] in conjunction with the Si XII/Si XIII/Si XIV ionisation balance calculations of Arnaud and Rothenfug [31].

3. Experimental data

The experimental results were obtained from the DITE tokamak at the UKAEA Culham Laboratory [32]. This tokamak has major and minor radii of 1.2 m and 0.24 m respectively, a maximum toroidal field of 2.7 T and maximum toroidal current of 300 kA. The central electron density can be varied between about $N_e \approx 5 \times 10^{12}$ and $\leq 10^{14}$ cm$^{-3}$, and the central electron temperature between about 500 and 1000 eV. Small concentrations (typically 0.01% of $N_e$) of Si ions were added to the plasma by sputtering from samples placed in the scrape-off layer by an adjustable probe. The central-chord integrated electron density was measured with a microwave interferometer [32], while radial profiles of electron density and temperature were determined by Thomson scattering of a 2 J ruby laser [33].

Most of the spectra were recorded with a Bragg rotor spectrometer [34], which had absolute calibration for flux and wavelength, and used a slotted (Soller) collimator to achieve a resolving power ($\lambda/\delta\lambda$) of about 600. Further Si XIII spectra, resolved to about 1 part in 2400 (limited by thermal doppler broadening), were recorded on Kodak DEF film with a curved crystal Johann spectrometer [35]. These better resolved spectra allowed an estimate of the contribution of satellite lines to the Si XIII spectrum, and were used to correct the R and G ratio measurements (see below).

The present results were recorded over almost the full density range of DITE so that at each density the ions could be observed in the centre of the plasma, where there is approximate coronal equilibrium. Radial profiles of the Si XIV/Si XIII emission ratio gave good agreement with coronal equilibrium for radii less than about 10 cm. Examination of the spatial Si XIII emission profile showed that almost all of the emission is from the central region of the plasma, where $N_e$ is almost constant and $T_e$ does not vary significantly. The range of $N_e$ and $T_e$ from which the central-chord signal is emitted is similar to the error in the measurement of the central values, i.e. about 10% for $T_e$ and 5% for $N_e$. This localisation of the emission allows the R and G ratios to be measured from the central-chord integrated signal alone, without the need for radial profiles at every plasma density.

The contribution of unresolved satellites was estimated from the high resolution spectra, which showed that there are significant satellites blended in the less well resolved spectra from which the R and G ratios were measured. The strongest dielectronic satellites at 6.74 Å are effectively unresolvable from the forbidden line, and their contribution has been calculated to be 13% of the observed forbidden line [36]. The satellite contribution to the intercombination lines is only a few percent and is less significant.

4. Results and discussion

Using the statistical equilibrium code of Dufton [37] with the atomic data discussed in Section 2, relative level populations and hence emission line strengths for Si XIII were estimated, where the following assumptions were made: (i) that photoexcitation and de-excitation rates are negligible in comparison with the corresponding collisional rates, and (ii) that all transitions are optically thin. Further details of the procedures involved may be found in Dufton [37].

In Figure 1 the theoretical R ratio is shown for values of electron density ($N_e \approx 10^{12} - 10^{15}$ cm$^{-3}$) typical of tokamak plasmas, at several temperatures between log $T_e = 6.4$ and 7.2, where Si XIII has a significant abundance in ionisation equilibrium [31]. The potential usefulness of the ratio as a density diagnostic is clear from the figure, as it varies by approximately a factor of 16 between log $N_e = 12.0$ and 15.0. Furthermore, it is relatively insensitive to electron temperature with, for example, a factor of 4 change in $T_e$ resulting in a 30% or less variation in R.

The sensitivity of R to recombination processes is illustrated in Figure 2, where the ratio is plotted as a function of $N_e$ at the temperature of maximum Si XIII emissivity, log $T_m = 7.0$ [38]. It can be seen that the effect of recombination on R is quite small, increasing its value by only about 10% in the low density limit.
The theoretical G ratio is plotted in Figure 3 as a function of electron temperature at a density \( N_e = 10^{13} \text{ cm}^{-3} \). We note that although G becomes density sensitive at high values of \( N_e \), decreasing due to quenching of the two photon \( 1s^2 \, ^1S - 1s2s \, ^1S \) transition by collisional excitation of \( 1s2s \, ^1S \) to the \( 1s2p \, ^1P \) state [39], this is not the case for the densities considered in the present analysis. For example, at \( \log T_e = 7.0 \) the values of G are 0.72 and 0.71 for \( \log N_e = 12.0 \) and 15.0 respectively. An inspection of Figure 3 shows that the effects of recombination on G are much larger than on R, increasing the former by approximately 25% at \( \log T_e = 6.8 \) and 60% at \( \log T_e = 7.2 \).

In Table 1 we compare the theoretical and observed values of R and G, and the comparison is also shown graphically in Figures 2 and 3. (We note that the observed electron temperatures all lie within 0.1 dex of \( \log T_e = 7.0 \), and as R is not strongly dependant on \( T_e \) (see above), it is hence justifiable to plot the experimental R ratios on one R vs. \( \log N_e \) curve). The high resolution data, obtained over limited \( N_e \) conditions but constant \( T_e \), were used to correct the low resolution observations for the presence of satellites over the larger range of \( N_e \) conditions. In Table 1 the uncorrected and corrected R ratios are labelled \( R_{\text{obs}} \) and \( R'_{\text{obs}} \) respectively, and the latter have been used in Figure 2. However we note that applying the same technique to the G ratio left it effectively unchanged, as the \( n > 3 \) satellites close to and under the resonance line contribute proportionally the same as the satellites under the forbidden and intercombination lines at these electron temperatures. Hence only the uncorrected G ratios \( G_{\text{obs}} \) are listed in Table 1.

An inspection of Table 1 and Figures 2 and 3 reveals that the agreement between the experimental and theoretical results is excellent, with discrepancies of typically 8% and 5% in R and G respectively. This provides support for the accuracy of the atomic data adopted in the line ratio calculations. The theoretical results may therefore be applied with confidence to the analysis of remote sources for which

![Figure 1](image_url)  
**Figure 1:** The theoretical emission line ratio R plotted as a function of electron density at electron temperatures of (from bottom to top), \( \log T_e = 6.4, 6.6, 6.8, 7.0, \) and 7.2, with dielectronic and radiative recombination and innershell ionisation included in the calculations.

<table>
<thead>
<tr>
<th>( N_e/10^{13}\text{cm}^{-3} )</th>
<th>( T_e/\text{eV} )</th>
<th>No. of spectra</th>
<th>( R_{\text{obs}} )</th>
<th>( R'_{\text{obs}} )</th>
<th>( R_{\text{theory}} )</th>
<th>( G_{\text{obs}} )</th>
<th>( G_{\text{theory}} )</th>
</tr>
</thead>
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<td>2</td>
<td>1.59</td>
<td>1.42</td>
<td>1.63</td>
<td>0.71</td>
<td>0.74</td>
</tr>
<tr>
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<td>3</td>
<td>2.13</td>
<td>1.94</td>
<td>2.03</td>
<td>0.73</td>
<td>0.73</td>
</tr>
<tr>
<td>9.0</td>
<td>700</td>
<td>3</td>
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<td>1.13</td>
<td>1.01</td>
<td>0.92</td>
<td>0.76</td>
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<tr>
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<td>750</td>
<td>4</td>
<td>1.86</td>
<td>1.68</td>
<td>1.92</td>
<td>0.74</td>
<td>0.74</td>
</tr>
<tr>
<td>1.2</td>
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<td>2</td>
<td>2.23</td>
<td>2.03</td>
<td>2.12</td>
<td>0.72</td>
<td>0.71</td>
</tr>
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<td>2</td>
<td>1.43</td>
<td>1.27</td>
<td>1.26</td>
<td>0.84</td>
<td>0.77</td>
</tr>
</tbody>
</table>

Table 1: Comparison of observed and theoretical Si XIII R and G ratios. \( R_{\text{obs}} \) and \( R'_{\text{obs}} \) are the observed values of R uncorrected and corrected for the presence of satellite lines, respectively.
Figure 2: The theoretical emission line ratio $R$ plotted as a function of electron density at the temperature of maximum Si XIII emissivity, $\log T_m = 7.0$ [38], with dielectronic and radiative recombination and innershell ionisation either included in (solid line) or excluded from (dashed line) the calculations. Typical errors in the experimental data (solid points) are $\pm 9\%$ in $R_{\text{obs}}$ and $\pm 0.02$ in $\log N_e$.

Figure 3: The theoretical emission line ratio $G$ plotted as a function of electron temperature at an electron density of $\log N_e = 13.0$, with dielectronic and radiative recombination and innershell ionisation either included in (solid line) or excluded from (dashed line) the calculations. Typical errors in the experimental data (solid points) are $\pm 6\%$ in $G_{\text{obs}}$ and $\pm 0.04$ in $\log T_e$.

no independent estimates of $N_e$ and $T_e$ exist, such as the solar flare x-ray spectra obtained with the P78-1 and Solar Maximum Mission satellites [14].

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