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PROTON EXCITATION OF THE $2s^22p^5 \, 2P_{3/2} - 2s^22p^5 \, 2P_{1/2}$ TRANSITION IN FLUORINE-LIKE Ti XIV and Ni XX

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Abstract: Rate coefficients for excitation of the $2s^22p^5 \, 2P_{3/2} - 2s^22p^5 \, 2P_{1/2}$ transition in fluorine-like Ti XIV and Ni XX by proton impact have been calculated using the close-coupled impact parameter method. These data are significantly different from earlier results with, for example, our proton rates for Ti XIV being approximately a factor of five smaller than those of Bely and Faucher (1970) at low temperatures. We show that the $2s^22p^5 \, 2P_{3/2} - 2s^22p^5 \, 2P_{1/2}$ transition in Ti XIV and Ni XX may be used to infer the electron density or ion temperature of a laboratory plasma through the diagnostic emission line ratios $R_1 = I(2s^22p^5 \, 2P_{3/2} - 2s^22p^5 \, 2P_{1/2})/I(2s^22p^5 \, 2P_{3/2} - 2s^22p^6 \, 2S_{1/2})$ and $R_2 = I(2s^22p^5 \, 2P_{3/2} - 2s^22p^5 \, 2P_{1/2})/I(2s^22p^5 \, 2P_{1/2} - 2s^22p^6 \, 2S_{1/2})$, although the theoretical values of $R_1$ and $R_2$ are strongly dependent on the magnitude of the proton excitation rate for $2s^22p^5 \, 2P_{3/2} - 2s^22p^5 \, 2P_{1/2}$. The accurate calculation of this quantity for Ti XIV and Ni XX is therefore of great importance.

1. Introduction

Emission lines arising from transitions in fluorine-like ions are frequently observed in the spectra of astronomical and laboratory plasmas [1-6]. Several authors have noted that the line ratios $R_1 = I(2s^22p^5 \, 2P_{3/2} - 2s^22p^5 \, 2P_{1/2})/I(2s^22p^5 \, 2P_{3/2} - 2s^22p^6 \, 2S_{1/2})$ and $R_2 = I(2s^22p^5 \, 2P_{3/2} - 2s^22p^5 \, 2P_{1/2})/I(2s^22p^5 \, 2P_{1/2} - 2s^22p^6 \, 2S_{1/2})$ in these ions should be of great use as electron density diagnostics [7-11], although to calculate $R_1$ and $R_2$ accurately, reliable atomic physics data must be employed, especially for the oscillator strength and electron and proton impact excitation rates between the $2s^22p^5 \, 2P_{3/2}$ and $2s^22p^5 \, 2P_{1/2}$ levels [12]. The proton rates are of particular importance as they tend to dominate the total collision rate at high temperatures [13].

Recently Keenan and Reid [14] have calculated proton excitation rates for the $2P_{3/2} - 2P_{1/2}$ transition in F-like Fe XVIII using the close-coupled impact parameter method [15]. They found these to be approximately a factor of 2.5 smaller than the results of Kastner and Bhatia [16], which hence lead to theoretical $R_1$ and $R_2$ diagnostic line ratios significantly different from those previously estimated [12]. In this paper we extend the Keenan and Reid work to derive proton rates for the F-like ions Ti XIV and Ni XX, and compare these with earlier calculations.

2. Proton excitation rate calculations

The proton excitation cross sections were calculated using the close-coupled semiclassical method which has been employed previously by many authors [14, 15, 17-22]. (For reviews of the semiclassical method and its relation to more accurate, quantal calculations, see Dalgarno [23] and Reid [24]. For the interaction, we have used the quadrupole interaction, modified at short range by use of a scaled-hydrogenic form of $r_2^2 r_3^3$, where $r_2$ and $r_3$ are the lesser and greater of the radius of the 2p electron and the ion-proton separation [21].

Our aim is for accuracy of about 10% in the cross sections and so we have omitted elaborations such as polarization effects [25], symmetrization of the coupled equations [19,20], or departures from LS-coupling [19,20]. The effects of these omissions, and of using a semiclassical rather than a quantal treatment of the collision have been discussed by Keenan and Reid [14] and Reid [24].

The excitation rate coefficients are derived by convolving the calculated cross sections with a Maxwellian energy distribution, and this requires cross sections at energies below those at which...
close-coupled calculations were made. These low energy cross sections were calculated by the symmetrized, first-order, semiclassical theory [26]. In the transition region, the discrepancy between the unsymmetrized close-coupled cross sections and the symmetrized first-order cross sections is less than 10%.

The excitation energies (in cm⁻¹) used in our calculations are 4.72 × 10⁴ for Ti XIV [27] and 1.44 × 10⁵ for Ni XX [28]. Expectation values <r²>₂p (in a₀) used in the calculations are 0.09438 and 0.05268 for Ti XIV and Ni XX respectively [29].

3. Results and discussion

In Figure 1 rate coefficients C (in cm³s⁻¹) for proton excitation of the 2s²2p⁵ ²P₃/₂ - 2s²2p⁵ ²P₁/₂ transition in Ti XIV and Ni XX are illustrated for a range of temperatures over which the ions have a fractional abundance in ionisation equilibrium of ≥ 10⁻² [30]. Also shown in the figure are the results of Bely and Faucher [13] for Ti XIV, as well as the calculations of Bhatia et al. [10] and Feldman et al. [9] for Ti XIV and Ni XX respectively. It can be seen that the present excitation rates are in good agreement with the Bhatia et al. and Feldman et al. data at the temperatures for which they quote results (T = 4 × 10⁶ K and 1 × 10⁷ K for Ti XIV and Ni XX respectively), but there are large discrepancies with the Bely and Faucher calculations for Ti XIV, where our estimates are more than a factor of five smaller at low temperatures, and up to 60% smaller at high temperatures. This latter discrepancy is expected, since it is known that modified first-order methods, such as the unitarized approximation used by Bely and Faucher, over-estimate the cross section for energies where the cross section is maximum [18,24,31]. However the large discrepancy at low temperatures is puzzling, since the rates at such low temperatures are determined by cross sections in the energy range where the first-order approximation is valid.

To illustrate the effects of the new proton rates on diagnostic line ratios for F-like ions, we have calculated the emission line ratio R₁ = I(2s²2p⁵ ²P₃/₂ - 2s²2p⁵ ²P₁/₂)/I(2s²2p⁵ ²P₃/₂ - 2s²2p⁵ ²S₁/₂) = I(694.54 Å)/I(83.18 Å) in Ni XX using the statistical equilibrium code of Dufton [32]. The model ion consisted of the 2s²2p⁵ ²P₃/₂, ²P₁/₂ and 2s²2p⁵ ²S₁/₂ states, the energies of these being taken from Corliss and Sugar [28], while for Einstein A-coefficients and electron impact excitation rates the atomic data of Feldman et al. [9] and Blaha [33,34] respectively were adopted. In Figure 2 the R₁ ratio is plotted as a function of electron density, where the four curves correspond to the ²P₃/₂ - ²P₁/₂ proton rate in the calculations being set equal to zero, or the present calculations at ion temperatures of

![Figure 1: Plot of the logarithmic proton excitation rates log C (C in cm³s⁻¹) for the 2s²2p⁵ ²P₃/₂ - 2s²2p⁵ ²P₁/₂ transition in F-like Ti XIV and Ni XX against log T (T is temperature in K), with: solid lines — the present calculations; dashed line — the atomic data of Bely and Faucher [13] for Ti XIV; cross — the calculation of Bhatia et al. [10] for Ti XIV; solid point — the calculation of Feldman et al. [9] for Ni XX.](image-url)
Figure 2: The theoretical Ni XX emission line ratio (in photons) $R_1 = I(694.54 \text{ Å})/I(83.18 \text{ Å})$ plotted as a function of electron density at the electron temperature of maximum Ni XX fractional abundance in ionisation equilibrium, $T_e = T_{\text{max}} = 6.3 \times 10^6 \text{ K}$ [30], with: solid line — proton excitation excluded from the calculations; short dashes line — proton excitation included using the present calculations at an ion temperature $T_{ion} = T_e/2$; long dashes line — proton excitation included with $T_{ion} = T_e$; dash-dot line — proton excitation included with $T_{ion} = 2T_e$.

$T_{ion} = T_e$, $T_e/2$ and $2T_e$, where the electron temperature $T_e$ is that of maximum Ni XX fractional abundance in ionisation equilibrium, $T_e = T_{\text{max}} = 6.3 \times 10^6 \text{ K}$ [30]. In all cases we have assumed that the proton density $N_p = N_e$. We note that the ratio $R_2 = I(2s^22p^5 \, ^2P_{3/2} - 2s^22p^5 \, ^2P_{1/2})/I(2s^22p^5 \, ^2P_{1/2} - 2s2p^6 \, ^2S_{1/2}) = I(694.54 \text{ Å})/I(94.50 \text{ Å})$ has the same density dependence as $R_1$ but with:

$$R_2/R_1 = 2.91$$ (1)

An inspection of Figure 2 shows that the $R_1$ ratio is strongly dependent on the value of the proton excitation rate for $2s^22p^5 \, ^2P_{3/2} - 2s^22p^5 \, ^2P_{1/2}$ and, hence, the ion temperature. The $R_1$ ratio may therefore be used to determine the ion temperature of a plasma if the electron density and temperature have been independently determined, as noted by, for example, Sato et al. [11] in the case of F-like Fe XVIII. Alternatively, if the ion temperature is known the ratio may be employed as an electron density diagnostic, as it is $N_e$-sensitive over the typical range ($N_e \approx 10^{13} - 10^{14} \text{ cm}^{-3}$) found in tokamak plasmas [35].

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