X-RAY LINE INTENSITIES FOR IONS OF THE HELIUM
ISOELECTRONIC SEQUENCE IN HIGH TEMPERATURE PLASMAS

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Helium Isoelectronic Sequence in High Temperature Plasmas

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Abstract

Measurements are reported for the He-like X-ray spectra of argon obtained in a deuterium tokamak plasma with \( N_e = 1-2 \times 10^{14}\) cm\(^{-3}\) and \( T_e = 1-2\) keV. The results are interpreted with the help of computed excitation rates and other available atomic data. The plasma sensitivity of line intensity ratios is discussed as well as the Z-dependence based on earlier observations of He-like S and Cl.

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The X-ray n=2 to n=1 spectrum of ions in the helium iso-electronic sequence consists of four principal lines conventionally labelled w, x, y, and z. These are associated with the n=2 states 2^1P, 2^3P, and 2^3S, respectively (the 2^3P state has no ground state transition and the 2^1S state decays by two-photon emission) (see Fig. 1). In a high temperature plasma, these states are mainly populated through electron impact excitation of the ground state 1^1S with cascade contributions from higher exited states. Owing to the long life time of the 2^3S state, the collisional excitation 2^3S -->2^3P, with a rate proportional to the electron density N_e, must also be considered. The presence of H-like and Li-like charge states in the plasma gives rise to recombination and ionization contributions in proportion to the ground state abundance ratio n_H:n_He:n_Li. For ion charge states in corona equilibrium, the n_H:n_He:n_Li ratios are calculable functions of β with the ratio β = T_e/T_m expressing the electron temperature T_e relative to the temperature (T_m) of maximum resonance-line emission. Excitation rates have been calculated by Pradhan et al.3,4) which together with available data for other processes have been used to derive relative intensities for the w, x, y, and z lines for different plasma conditions. In order to express the T_e and N_e dependences in the spectrum one defines the line intensity combinations G = (x+y+z)/w and R = z/(x+y), respectively, to which X = x/y can be added as the third plasma independent line ratio. Auxiliary information on plasma conditions is provided by satellite lines to the He-like resonance transition due to states with a spectator electron in the 2p or 2s orbitals (see Fig. 1). The 2p states are formed by dielectronic recombination and the satellite to resonance intensity ratio D = s_d/w is a sensitive function of T_e in a limited temperature range for T_e < T_m but independent of the ion-charge state balance. The 2s states are formed by inner shell excitation so the line ratio I = s_1/w reflects the abundance ratio n_Li/n_He in the region of the He-like ions against which the corona equilibrium ratio at
given $\beta$ can be compared $^5$).

The intensities of both principal and satellite lines in the He-like spectrum are critically sensitive to the nuclear charge $Z$ since the rates of the radiative transitions depend on $Z$ and since the ion charge state distribution varies with $Z$ through $T_m = T_m(Z)$. As a consequence the plasma parameter sensitivity of the line ratios will change with $Z$. This is an important consideration for plasma diagnostics applications where it is desirable to maximize the response in the measured line ratios, for instance, $dR/dN_e$, $dG/dT_e$, etc., or for atomic rate studies in which case the plasma condition sensitivity might preferably be kept small. The $X$-ratio is an example of the latter category where the M2 rate of the ground state transition (line $x$) increases rapidly with $Z$ (in the context of excitation rates that are slowly varying with $Z$) to become equal to the El rate of the competing branch $2^3P_2 \rightarrow 2^3S_1$ for $Z$ between 18 and 19 $^6)$. For $Z > 20$ the departure from pure LS coupling begins to manifest itself in the excitation rate for the $2^3P_1$ level which becomes enhanced due to interaction with the $2^1P_1$ level (singlet-triplet mixing). The present work entails the spectra of ions below this limit ($Z < 20$). Therefore, all $2^3P$ population rates divide between the fine structure components according to statistical weights and the ratio $x = x/y$ is entirely fixed by the radiative branching decay rates. Although there are a number of laboratory and astrophysical observations of the line spectra of He-like ions, no experimental study has been done of the systematic variation of the line intensities with nuclear charge. In this paper we present the results of such an investigation based on new measurements for Ar and our earlier measurements for S and Cl for similar plasma conditions.
The experiment was carried out at the MIT Plasma Fusion Center on the Alcator C tokamak. The X-ray emission from the tokamak plasma was measured with a Bragg crystal spectrometer of the van Hamos geometry using position sensitive proportional counters for the photon detection; some high count rate discharges were observed with the new delay line detector described in ref. 8 (an example is shown in Fig. 2). The deuterium plasma with typical parameters of \( N_e = 1-2 \times 10^{14} \text{ cm}^{-3} \) and \( T_e = 1-2 \text{ keV} \) was seeded with argon to concentration levels of \( 10^{-5} \) to \( 10^{-4} \) relative to \( N_e \). The plasma was practically unaffected by the seeding and yet allowing the measurement of He-like spectra with good statistics for individual plasma discharges; actually, the Ar concentration could be controlled (in contrast to previous experiments using the ambient impurity species sulphur and chlorine) and adjusted up to the level permitted by the data rate capabilities of the electronics. At a spectrometer Bragg angle of \( \Theta_B = 28.0^\circ \) we covered a bandwidth of \( \lambda = 3.9-4.4 \text{ Å} \) with the He-like Ar spectrum lying in the range \( \lambda = 3.95-4.05 \text{ Å} \). The plasma conditions were monitored with standard diagnostic methods giving information on \( N_e \) and \( T_e \).

In the He-like spectrum of argon (Fig. 2) we see the four principal lines \( w, x, y, \) and \( z \) as well as the lines \( k \) and \( q \) representing \( s_d \) and \( s_i \) satellites, respectively (see Fig. 1 for definition of letter symbols). Two other weaker satellites \( (r \) and \( a, \) representing \( s_i + s_d \) and \( s_d \) intensities) can also be identified along with satellites due to spectator electrons in \( n > 3 \) orbitals appearing as foothills near the resonance line. Estimates for satellite contributions were obtained from calculated \(^1,9\) intensity ratios using the measured \( k \) and \( q \) lines as references for normalizing \( s_d \) and \( s_i \) intensities. Hence the \( j \)-line intensity can be subtracted from the blended \( j+z \) peak allowing the \( z \)-line intensity to be determined. Our measurements thus provide line intensities for the \( x, y, z, q, r, a, \) and \( k \) lines relative to the resonance line.
for individual plasma discharges with the principal parameters $N_e$ and $T_e$ obtained from other diagnostic measurements. An example is shown in Fig. 2 which refers to the X-ray emission collected over 100 ms of the constant current ($I_p = 450$ kA) portion of a plasma discharge. Our data consist of spectra from several hundred discharges. In order to mitigate the shot-to-shot variations (discussed in ref. 7) and to improve counting statistics, we determined average line intensities representing a plasma with $N_e = 1.5 \times 10^{14}$ cm$^{-3}$ and $T_e = 1.4$ keV. The results on average line intensities for argon (along with earlier results for sulphur and chlorine$^7$) are given in Table 1. Comparison is made with theoretical intensity ratios obtained in the following manner.

Corona equilibrium calculations for Ar were carried out, employing the excitation rate coefficients by Pradhan et al.$^{3,4)}$. The main atomic processes included are excitations and cascades along with radiative and dielectronic recombination. In addition, the $\zeta_{\pi\gamma}$ formula was used to estimate the small inner shell ionization contribution to the $\pi$ line$^4)$. Line intensity ratios were calculated for $T_e = 1.4$ keV compared to $T_m = 1.63$ keV for Ar. The ratio $G$ is a monotonically decreasing function of $T_e$ in the range $T_e < T_m$ due to the decrease in the recombination contribution, mainly for the triplet states, and the increase in resonance line emission with temperature. We obtain $d(\ln G)/dT_e \approx -0.23$ keV$^{-1}$ for our conditions. The ratio $R$ is most sensitive to the plasma parameter $N_e$ because of the collisional $2^3S_1 \rightarrow 2^3P_j$ transfer, the rate of which is proportional to $N_e$. The plasma sensitivity in this case is about $d(\ln R)/dN_e \approx 0.13 \times 10^{-14}$ cm$^3$. The calculated intensities for the principal lines are found to agree with the observations (Table 1) which lends support to the underlying theory and particularly the computed excitation rates.
In earlier works, the satellite to resonance line ratio was computed using an approximate rate coefficient (such as with a Gaunt factor) for the resonance line. However, accurate rates have now been computed explicitly by Pradhan et al.\(^3\) and therefore we derive, and employ, the following expression for these ratios:

\[
D = \frac{2.4 \times 10^{-11}}{T \gamma_w(T)} \left[ \frac{\epsilon_s A_a A_r}{\Sigma A_a + \Sigma A_r} \right] e^{(E_0 - E_s)/kT} \tag{1}
\]

where \(\gamma_w\) is the Maxwellian averaged collision strength and \(\epsilon_s\) is the statistical weight factor of the satellite state. In order to calculate \(D\), we used the auto-ionization and radiative probabilities \((A_a\) and \(A_r)\) computed by Vainshtein and Safronova\(^1\), which in the case of Ca and Fe have been found to agree to within a few percent with those of Bely-Dubau et al.\(^9,10\). We find that the \(D\) ratio is decreased by about 25% compared to earlier calculations because of the \(\gamma_w\) factor in Eq. 1, which is higher than the approximate rates previously used. The theoretical \(k/w\) ratio is calculated to be 0.058 for \(T_e = 1.4\) keV which is close to the observed ratio of 0.062; the temperature sensitivity is \(d(\ln D)/dT_e = 1.41\) (keV)\(^{-1}\) so the statistical uncertainty is, for instance, \(+150\) keV for the spectrum of Fig. 2. This result provides corroborating evidence that the observed emission comes from He-like Ar ions in a plasma of \(T_e = 1.4\) keV. With regard to the \(I\) ratio, the calculated \(q/w\) intensity ratio is 0.043 for \(T_e = 1.4\) keV and hence significantly smaller than the observed value of 0.061. If this result were to be interpreted in terms of the charge state balance, the corona equilibrium ratio \((n_{Li}/n_{He})_{cor}\) would have to be taken at an apparent (ionization) temperature of \(T_z = 850\) eV (i.e., \(T_z < T_e\)) in order to equate \((q/w)_{cor}\) and \((q/w)_{obs}\), with the charge state distribution being a function of \(\beta_z = T_z/T_m\). Using \(\beta_z\) for determining the \(n_H/n_{He}\) ratio would decrease the recombination contributions to the excitation
rates of the principal lines and subsequently decrease the calculated \( G \) and \( R \) ratios of Table 1 by about 9%. The cause of the difference \( T_e \neq T_z \) might be ascribed to charge state balance effects because of differences in the spatial distribution of the H-, He- and Li-like ions in a limited size plasma of a tokamak (see below). The fact, however, that unexpectedly high \( q/w \) intensity ratios have been found for various ions in tokamak plasmas as well as astrophysical plasmas suggest to us that the theoretical excitation rates used are rather crude approximations (cf. the rates for the He-like ions mentioned above) giving too low values for Li-like relative to He-like ions. Therefore, our results on the \( q/w \) ratio indicates the need for more accurate excitation rates for Li-like ions rather than suggesting that \( T_z \neq T_e \).

In Table 1, comparison can be made between X-ray line ratios for He-like spectra of sulphur, chlorine and argon. For all three ions we are in a density regime where \( R \) is density dependent and \( R \ll R_o \), the low density limit. Theoretically, for fixed electron density, the value of \( R \) should increase with \( Z \) as it approaches the maximum value \( R_o (Z) \). The temperature dependence of the ratio \( G \) is such that for most He-like ions \( G(T_m) \) lies in the range 1.0–0.7 and \( G(T) \gg G(T_m) \) for \( T \ll T_m \). In the present case, for a temperature of \( T \approx 1.4 \text{ keV} \), \( G \) is expected to show some increase with \( Z \) since \( T \gg T_m \) for S and \( T \ll T_m \) for Ar. We note in particular the \( Z \)-dependence for the principal line which is predicted to be \( \frac{d(\ln R)}{dZ} = 0.23 \), \( \frac{d(\ln G)}{dZ} = 0.05 \) and \( \frac{d(\ln X)}{dZ} = 0.27 \) for constant plasma conditions. This is found to account for the data in Table 1 typically to within \( \pm 15\% \) which is not outside the experimental uncertainties. In order to put the theory to a more stringent test, the plasma conditions must be better specified, particularly with respect to radial profiles which vary with \( Z \) depending on \( T_m (Z) \) relative to \( T_e \). These effects can be assessed and the related uncertainties in line intensities...
reduced by simultaneously measuring spectra for different ion species where the temperature of the discharge is varied around the $T_m$-values given. Furthermore, we note the predicted increase in the X ratio with Z, which accounts for the observed values in the range $Z = 16-18$. For $Z > 20$, the ratio X would depend on plasma parameters and should be lower than if the ratio were to be computed as for $Z < 20$. Other data\textsuperscript{10-13} for He-like ions with $Z > 20$ (for instance, Ca, Ti, Cr, and Fe) tend to show a less pronounced Z dependence which in part would signal the onset of spin-orbit coupling. The importance of intermediate coupling effects in connection with auto-ionization and dielectronic recombination contributions to excitation rates is presently being investigated\textsuperscript{14} for ions up to $Z = 42$ using extensive 9-state calculations.

In conclusion, our new measurement of the He-like spectra of argon along with previous data on sulphur and chlorine exhibit line intensity ratios of a systematic variation along the helium isoelectronic sequence. The principal line intensities can be accounted for with the help of computed (ab initio) excitation rates and available data for atomic decay rates. Using the calculated rate for the resonance line we derive an electron temperature from the observed dielectronic satellite to resonance line intensity that agrees with the independently diagnosed value. Our results thus support the theoretical atomic rates involving the $n=1$ and $n=2$ He-like states which furnish the basis for X-ray spectroscopic diagnostics of both laboratory and astrophysical plasmas. In contrast we find that the excitation rate for Li-like argon (and other medium Z atoms) need to be checked before the ratio of inner shell excitation satellite to resonance line intensities can be used as a reliable measure of the Li-like to He-like abundance ratio and hence an indicator of the ion charge state balance.
It is a pleasure to acknowledge the support of R. Parker and the Alcator group and for providing for the argon seeding of the plasma need for this experiment. This work was supported by the U.S. Department of Energy and by the National Sciences and Engineering Research Council of Canada.
Table 1  Intensity ratios for lines in the He-like spectrum of argon (present experiment), chlorine and sulphur (from ref. 7). The theoretical values are for plasma conditions of $N_e = 1.5 \times 10^{14} \text{cm}^{-3}$ and $T_e = 1.4$ keV in the case of Ar and $N_e = 3 \times 10^{14} \text{cm}^{-3}$ and $T_e = 1.3$ keV in the case of S and Cl.

\[
\begin{array}{ccccccc}
\hline
& x/w & y/w & z/w & G & R & X \\
\hline
\text{Ar} & \text{Exp.} & 0.15 & 0.20 & 0.41 & 0.75 & 1.21 & 0.79 \\
& \text{Theory} & 0.15 & 0.19 & 0.46 & 0.81 & 1.30 & 0.80 \\
\text{Cl} & \text{Exp.} & 0.17 & 0.25 & 0.39 & 0.81 & 1.04 & 0.69 \\
& \text{Theory} & 0.16 & 0.24 & 0.43 & 0.83 & 1.08 & 0.65 \\
\text{S} & \text{Exp.} & 0.16 & 0.29 & 0.41 & 0.85 & 0.97 & 0.55 \\
& \text{Theory} & 0.15 & 0.29 & 0.34 & 0.78 & 0.77 & 0.52 \\
\hline
\end{array}
\]
References


14) A.K. Pradhan (to be published).
Figure Captions

Figure 1: Term diagram for the He-like n=2 to n=1 spectrum of argon showing the X-ray lines seen in this experiment with the wavelengths from refs. 1 and 2.

Figure 2: The He-like spectrum of argon for a single plasma discharge characterized by $N_e = 1.7 \times 10^{14} \text{ cm}^{-3}$ and $T_e = 1.6 \text{ keV}$ the toroidal field being 80 kG and the current 450 kA. The X-ray lines are identified by conventional letter symbols (see text) and their wavelength positions marked as predicted$^{1,2}$ relative to the w and z lines.