The Rydberg series of helium-like Cl, Ar and S and their high-$n$ satellites in tokamak plasmas

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Abstract. The Rydberg series up to $n = 14$ of helium-like chlorine, argon and sulfur have been observed in Alcator C-Mod plasmas. High-$n$ satellites to these lines of the form $1s^22s–1s2sp$ and $1s^22p–1s2np$ with $3 \leq n \leq 12$ have also been seen for chlorine and argon. Accurate wavelengths of these satellites have been obtained, comparison has been made with the theoretical predictions from the atomic structure codes RELAC and MZ, and the agreement is good. Measured line intensities have also been compared with collisional radiative modelling that includes the contributions from dielectronic recombination and inner-shell excitation rates to each line’s emission, again with good agreement.

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1. Introduction

X-ray spectroscopy is often applied to diagnose plasma conditions in high-density inertial confinement fusion capsule implosions [1]–[5] and in the laser-produced plasmas surrounding the capsule [6, 7]. In order to produce the required radiation, high-Z impurities (usually Ar) are added as trace dopants (≤0.2%) to the deuterium fuel capsules. Due to the high temperatures of these laser-produced plasmas, H-, He- and Li-like ions are produced abundantly; due to the very high densities in these plasmas, the Lyα and Heα line transitions are often optically thick. Thus, higher-energy (higher-\(n\)) transitions are required to extract information about the local plasma conditions. Stark broadening of the Heβ resonance line of Ar16+ is used for density determination [8]. The ratio of the Heβ and Lyβ emission from Ar16+ and Ar17+, respectively, is used to infer the fuel temperature [9]–[11]. The ratio of intensity in Kβ Ar15+ dielectronic satellite lines to the Heβ resonance line is a sensitive temperature diagnostic [12]; the satellite features blend with the Heβ line, and need to be included self-consistently in the fit of the whole lineshape with a Stark broadening code coupled to a kinetics (collisional–radiative) model [13]–[15]. To this end, unambiguous observations of high-\(n\) He-like resonance transitions and the associated Li-like satellites are crucial for developing and benchmarking atomic models. High spectral resolution measurements of K-shell Ar and Cl emission features from tokamak plasmas provide exactly the clean data needed to proceed.

In lower-density, magnetically confined fusion plasmas the very high-\(n\) members of the He-like resonance series (e.g. \(n = 10\) for Ar16+) are directly populated by charge-exchange recombination with neutral deuterium in the ground state. Spatially resolved measurements of this line can be used to map directly the neutral particle distribution in the plasma. Recent work by Rosmej [16] has shown that the ratio of the resonance and intercombination components of the Heβ transition in argon is sensitive to cascading from highly excited triplet states, and charge-exchange recombination into highly excited He-like levels. Again, high-resolution x-ray spectra from well diagnosed plasmas are crucial for developing and benchmarking the models that will serve as plasma diagnostics. Specifically, study of the higher-\(n\) members of the He-like Rydberg series and their associated satellites is necessary to understand the charge-exchange recombination and radiative cascade processes in magnetically confined fusion plasmas. An isoelectronic study of these spectra is necessary in order to understand the problems of blending that may occur when higher-order members of a lower charge state overlap with lower-order members of the resonance lines in higher charge states.

The \(n = 2\) and \(3\) x-ray spectra from many mid- and high-Z He-like ions have been studied in tokamak plasmas [17]–[19] and in solar flares [20, 21]. The high-\(n\) Rydberg series of medium-Z helium-like ions have been observed from Z-pinch [22, 23], laser-produced plasmas [24], exploding wires [23], the solar corona [25], tokamaks [26]–[28] and ion traps [29]. Always associated with x-ray emission from these two-electron systems are satellite lines from lithium-like ions. Comparison of observed x-ray spectra with calculated transitions can provide tests of atomic kinetics models and structure calculations for helium- and lithium-like ions. From wavelength measurements, a systematic study of the \(n\) and \(Z\) dependence of atomic potentials may be undertaken. From the satellite line intensities, the dynamics of level population by dielectronic recombination and inner-shell excitation may be addressed.

Satellites to the Ar16+ Rydberg series for \(n = 2\) [26, 30], \(n = 3\) [23, 28] and \(n = 4, 5\) [26, 27] have been examined extensively. Theoretical calculations of \(n \geq 3\) satellites for argon (and other elements) are plentiful [27, 31]–[34]. For \(n \geq 6\) satellites, some wavelengths have
been reported [23, 26, 27], and wavelengths and oscillator strengths have been calculated up to \( n = 7 \) [22, 23], but various wavelength calculations differ from the measured values by 3 mÅ. Observations for Cl\(^{15+} \) \( n = 2 \) transitions have been made in Alcator A [35], Alcator C [36], JET [37] and COMPASS-D [37] plasmas, and \( n = 3 \) transitions have been seen in laser-produced plasmas [24]. The diagnostic potential of He-like spectra for \( n = 3 \) and higher-\( n \) transitions has been exhaustively developed by Bely-Dubau et al [38, 39]. The use of inner-shell excited satellites as a measure of Li-like to He-like ion abundance is developed by Bely-Dubau et al in [40].

This paper is organized as follows. The code description and experimental set-up are given in section 2. Observations and code comparisons for the Rydberg series of helium-like Cl\(^{15+} \) between \( n = 3 \) and 14, and the high-\( n \) satellites of Cl\(^{14+} \) with \( 3 \leq n \leq 10 \) are presented in section 3. Similar results for argon are shown in section 4. The observed Rydberg series of S\(^{14+} \) and calculations, including S\(^{13+} \) satellites, are given in section 5.

2. Code descriptions and experiment

Ab initio atomic structure calculations for the lithium-, helium- and hydrogen-like isosequences of S, Cl and Ar \((Z = 16 - 18)\) with \( 2 \leq n \leq 14 \) have been generated using the HULLAC package. HULLAC includes ANGLAR, which uses the graphical angular recoupling program NJGRAF [41] to generate fine structure levels in a \( jj \)-coupling scheme for a set of user-specified electron configurations. HULLAC then generates atomic wavefunctions using the fully relativistic, parametric potential code RELAC [42, 43], which calculates the full multi-configuration, intermediate coupled level energies and radiative transition rates. RELAC also computes semi-relativistic autoionization transition rates [44] to the ground and excited levels of an adjacent ion. The CROSS [45] suite of codes in the HULLAC package uses the factorization theorem of Bar-Shalom, Klapisch and Oreg to compute the distorted-wave approximation electron-impact excitation rates between all levels of each charge state mentioned above. This includes levels formed by exciting valence-shell electrons as well as deeply bound inner-shell electrons.

Energy levels and transition probabilities have also been calculated by using the \( Z \)-expansion method (MZ code). The energy matrix is constructed in an \( LSJ \) coupling scheme and relativistic corrections are included within the framework of the Breit–Pauli operator using a perturbation approach. The MZ method uses hydrogenic wavefunctions. However, the calculation energies and other characteristics by this method are greatly improved by using many-body perturbation theory to include the Coulomb interaction between electrons as well as relativistic corrections. The \( Z \)-expansion method has been described in detail in [46, 47].

The ionic transition rates, including the autoionization rates from the Li- to He-like and He-like to H-like ions, as well as direct impact ionization (including ionization from valence- and inner-shell orbitals) and radiative recombination rate coefficients are used to construct the collisional–radiative rate matrix, \( R_{i \rightarrow j} \),

\[
\frac{dn_i}{dt} = \sum_i n_i R_{i \rightarrow j} - n_j \sum_i R_{j \rightarrow i} \tag{1}
\]

where \( n_j \) is the population in level \( j \) and \( R_{i \rightarrow j} \) is the total rate for transitions between level \( i \) and \( j \). The inverse of each ionization process, namely dielectronic recombination and three-body recombination has been found according to the principle of detailed balance. The bare nuclei
for S, Cl and Ar are also included in the rate matrix; the relative populations of the four charge states are found in the steady state by setting the time derivative of the population in each level equal to zero and inverting the matrix.

The lithium-like satellite transitions to the helium-like resonance lines considered here can be excited by two mechanisms, inner-shell electron impact excitation of the lithium-like ion,

$$1s^22l + e^- \rightarrow 1s2lnl' + e^-$$

or dielectronic recombination from the helium-like ion,

$$1s^2 + e^- \rightarrow 1s2lnl^* \rightarrow 1s^22l + \gamma$$

where $1s^2lnl^*$ is a singly or doubly excited autoionizing lithium-like level, $1s^22l$ is a stable lithium-like level and $\gamma$ is the observed photon. The emissivity of a line from level $j$ of ion $Z$ excited by electron impact excitation is given by

$$\varepsilon_{ex} = n_en_ZC_{ex}(T_e)\beta_{j,f}$$

where $n_e$ and $n_Z$ are the electron and ion densities, $C_{ex}(T_e)$ is the impact excitation rate coefficient and $\beta_{j,f}$ is the radiative branching ratio for the observed transition from level $j$ to level $f$. The inner-shell excitation channel makes a significant contribution to a lithium-like satellite line’s intensity only when the initial level is the lithium-like ground level. For the lines in the tables of sections 3 and 4 that end on excited levels of the lithium-like ion, the dominant excitation mechanism is via dielectronic recombination.

The emissivity $\varepsilon_{DR}$ of a lithium-like satellite excited by dielectronic recombination can be expressed as

$$\varepsilon_{DR} = n_en_{He}F_1(T_e)F_2(j,f)$$

where all the temperature dependence is contained in

$$F_1(T_e) = \frac{1}{2} \left( \frac{4\pi a_0^2 R}{T_e} \right)^{3/2} \exp\left(-\Delta E_{i,j}/T_e\right)$$

where $a_0$ is the Bohr radius, $R$ is the Rydberg unit of energy and $\Delta E_{i,j}$ is the energy of the captured electron. The satellite intensity factor due to dielectronic recombination from level $i$ of ion $(Z+1)^+$ through level $j$ of ion $Z^+$ to level $f$ is given by

$$F_2(j,f) = \frac{g_j}{g_i}A_{j,i}A^R_{j,f}$$

where the $g$s are the statistical weights of the intermediate (autoionizing) and initial (recombining) levels, $A_{j,i}^A$ is the rate of autoionization from level $j$ to level $i$, and

$$\beta_{j,f}^R = \frac{A^R_{j,f}}{\sum_i A_{j,i}^A + \sum_f A^R_{j,f}}$$

is the branching ratio for radiative stabilization for the observed transition. The sum over $i$ in equation (8) runs over all levels in the next higher ion reachable from level $j$ by autoionization, and the sum over $f$ runs over all bound levels reachable from $j$ by radiative decay. Radiative decays from level $j$ to other autoionizing levels have been neglected; stabilization following
transitions between continuum levels has a small effect on the computed branching ratio. All atomic data required for equation (5) have been generated ab initio with RELAC [43, 44].

A lithium-like dielectronic satellite line \((j \rightarrow f)\) and the corresponding helium-like resonance line \((w_n)\) can be used as a temperature diagnostic of the local plasma conditions by dividing equation (4) by (5),

\[
\frac{\varepsilon_{w_n}}{\varepsilon_{J,DR}} = \frac{C_{w_n}^{ex}(T_e)}{F_1(T_e)F_2(j,f)}
\]

where the branching ratio for the helium-like resonance line is assumed to be one, and recombination population of the upper levels of \(w_n\) has been ignored. For \(n = 2\), this ratio has been routinely used for electron temperature determination [36, 48]. The advantage of using these line ratios is that the result is independent of the helium-like charge state density.

The x-ray observations described in the following sections were obtained from the Alcator C-Mod [49] tokamak, a compact (minor radius \(a \sim 22\) cm, elongation \(\kappa \leq 1.8\)), high-field device with all-molybdenum plasma-facing components. All of the results here are for Ohmic deuterium plasmas, with the central plasma parameters in the range of \(0.9 \times 10^{20} \text{ m}^{-3} \leq n_{e0} \leq 1.8 \times 10^{20} \text{ m}^{-3}\) and \(900 \text{ eV} \leq T_{e0} \leq 2600 \text{ eV}\).

The x-ray spectra presented were recorded by a five-chord, independently spatially scannable, high-resolution spectrometer array [50]. Each spectrometer has a resolving power, \(\lambda/\Delta\lambda\), of 4000, a 2 cm spatial resolution and a luminosity function of \(7 \times 10^{-9} \text{ cm}^2 \text{ sr}\). Measured linewidths are usually dominated by Doppler broadening. Recently, one of the five spectrometers has been fitted with an ADP crystal, which has a \(2d\) spacing of 10.640 Å, to allow access to longer wavelengths. In the present paper, high-resolution x-ray observations in the wavelength range \(2.98 \text{ Å} \leq \lambda \leq 4.52 \text{ Å}\) are shown. Wavelength calibration [51] has been achieved after determining the instrumental dispersions with reference to H- and He-like argon, chlorine and sulfur lines and previously measured molybdenum [52] lines. Lines from hydrogen-like [53, 54] ions are taken to have precise wavelengths, either measured or calculated. The accuracy of measured wavelengths described here is \(\pm 0.3 \text{ mÅ}\), determined mainly from the quality of the line fits, and is less than the differences in various calculated Li-like wavelengths. The argon was puffed into the plasma through a piezo-electric valve and the chlorine was introduced by freon \((\text{C}_2\text{Cl}_3\text{F}_3)\) injection utilizing a fast scanning probe [55]. Chlorine is also present as an intrinsic impurity from solvents used to clean vacuum components. Presumably, sulfur is a trace impurity in the molybdenum.

3. Chlorine experimental observations and code comparisons

To provide adequate chlorine levels in the plasma, freon (tri-chloro-tri-fluoro-ethane) has been injected using the fast scanning probe. In figure 1 the time histories of the electron and chlorine densities, the electron temperature and the brightnesses of spectroscopic lines from fluorine \((\text{F}^{8+}, 883.1 \text{ Å})\) and chlorine \((\text{Cl}^{15+}, 4.44–4.50 \text{ Å})\) are shown for a discharge that had freon injections at 0.5 and 0.8 s. The impurity confinement for these halogens is very similar to that for other non-recycling impurities injected by laser blow-off into L-mode plasmas [56]. At the beginning of the discharge there is substantial intrinsic chlorine and fluorine (from solvents and exposed teflon) present until the plasma becomes diverted around 0.25 s, when impurity penetration drastically decreases [57]. The chlorine density has been determined from the brightnesses of the \(n = 2\)
Figure 1. The time histories of several parameters of interest for a discharge with freon injections at 0.5 and 0.8 s. Top part, electron (full green curve) and chlorine (chain red, \( \times 10^4 \)) densities; middle part, the central electron temperature and lower part, lithium-like (883 Å) fluorine (green) and helium-like (4.44–4.50 Å) chlorine (red) line brightnesses, on an arbitrary scale.

to 1 transitions [35]–[37] of \( \text{Cl}^{15+} \) in a similar fashion to the argon density measurements [58]. The electron density was measured by a two-colour interferometer and the electron temperature was determined from electron cyclotron emission measurements.

An x-ray spectrum in the vicinity of the \( n = 3 \) resonance line of \( \text{Cl}^{15+}, 1s^2 \ 1S_0–1s3p \ 1P_1 \) (w3), is shown in figure 2. The upper level is 0.75 \( (1s_{1/2}3p_{3/2})_1 + 0.25(1s_{1/2}3p_{1/2})_1 \) in \( jj \)-coupling notation. This admixture of the two \( J = 1 \) levels for 1snp has almost the exact same proportion (75:25) for all \( n \) values that have been checked \( (n \leq 14) \). Also visible in this spectrum is the intercombination line \( (y_3), 1s^2 \ 1S_0–1s3p \ 3P_1, \) at 3794.7 mÅ, and four groups of unresolved satellites denoted by \( A_3, B_3, A'_3 \) and \( C_3 \). \( A_3 \) and \( A'_3 \) have upper levels of the form 1s2p3p which are populated by dielectronic recombination of \( \text{Cl}^{15+} \), while \( B_3 \) and \( C_3 \) have upper levels of the form 1s2s3p which can either be populated by dielectronic recombination or inner-shell excitation of \( \text{Cl}^{14+} \). The brightest chlorine lines contributing to the spectrum of figure 2 are listed in table 1, which includes the transition designations (\( jj \)-coupling), calculated wavelengths from MZ and RELAC, satellite capture energies (as in equation (6)), oscillator strengths/satellite intensity factors (equation (7)) and (inner-shell) excitation rates (as in equation (4), evaluated at 1500 eV).

Shown for comparison in the lower part of figure 2 is a synthetic spectrum, generated with the calculated wavelengths from RELAC, Doppler (and instrumental) linewidths and intensities from the collisional radiative model described above. The line intensities are determined from

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Figure 2. The observed x-ray spectrum of the helium-like Cl\textsuperscript{15+} resonance line \(w_3\) with the intercombination line \(y_3\) and satellites is shown on a linear scale in the top part. In the bottom part is a log plot, including a simulated spectrum with \(w_3\) and \(y_3\) shown in green and the satellite groups shown in red.

the emissivities of equations (4) and (5), using measured electron temperature and density profiles, with charge state density profiles calculated from the impurity transport code MIST [59] (including the appropriate impurity transport coefficients [56]). The line brightness is then determined by integrating the emissivity profile along the observation line of sight for each transition. The observed spectrum was obtained from a plasma which had a central electron temperature of 1200 eV and a central electron density of \(1.8 \times 10^{20}\) m\(^{-3}\). The agreement between the calculated and the observed spectra is good. There is strong configuration interaction in the RELAC calculations between the 1s2p3p upper levels of the \(A_3\) and \(A'_3\) transitions and the 1s2s3s and 1s2s3d levels. Here the configuration interaction ‘pushes up’ or raises the 1s2p3p level energies. When the configuration interaction is turned off, the calculated wavelengths for the transitions making up \(A_3\) and \(A'_3\) increase by about 3.5 mÅ (these shifted wavelengths are what is plotted in figure 2). This interaction is seen to diminish rapidly with increasing \(n\).

Molybdenum lines [52] at 3785.7, 3831.0 and 3834.6 mÅ contaminate this spectrum. While the relative intensities calculated for the satellites are in good agreement, the predicted intensity for the intercombination line \(y_3\) is too low. The observed ratio of \(y_3/w_3\) is \(~0.05\), while the calculated value is \(~0.030\). This has also been observed in argon [27]–[29] and iron [60]. There is a predicted feature at 3810.5 mÅ that is due to lithium-like transitions of the form 1s\(^2\)3\(l\)–1s3\(l'\)). These satellites to the \(w_3\) and \(y_3\) lines are fed almost exclusively by dielectronic recombination from the ground level of Cl\textsuperscript{15+}, although some of the low-lying excited levels of
Table 1. The Cl\textsuperscript{15+} \(n = 3\) resonance and intercombination lines, with Cl\textsuperscript{14+} satellites. The transition designations (the largest basis function in the intermediate-coupling calculation), calculated wavelengths, satellite capture energies, oscillator strengths/satellite intensity factors and inner-shell excitation rates (at 1500 eV) are given for the strongest lines. In the third and fourth columns are the calculated wavelengths, in mA, from the MZ and RELAC codes, respectively. The satellite capture energies (from RELAC) in the fifth column are in eV. For the resonance and intercombination lines, the entries in the sixth column are the oscillator strengths (from RELAC), while for the satellites, the rates (at 1500 eV) are given for the strongest lines. In the third and fourth columns are the calculated wavelengths, in mÅ, from the MZ and RELAC codes, respectively. The satellite capture energies (from RELAC) in the seventh column are cm\(^3\) s\(^{-1}\). Powers of 10 are given in brackets, [ ].

| Line | Transition | \(\lambda_{MZ}\) (mÅ) | \(\lambda_{rel}\) (mÅ) | \(g^*f\) | \(C_{ex}\) (cm\(^3\) s\(^{-1}\)) |
|------|------------|----------------------|----------------------|--------|---------------------|
| \(w_3\) | 1s\(^2\) 1S\(_0\)–1s3p \(^3\)P\(_1\) | 3789.9 | 3789.6 | 1.635[−1] | 4.275[−13] |
| \(y_3\) | 1s\(^2\) 1S\(_0\)–1s3p \(^3\)P\(_1\) | 3794.3 | | 1.490[−3] | 6.459[−14] |
| \(A_3\) | 1s\(^2\) 1S\(_0\)–1s3p \(^3\)P\(_1\) | 3838.1 | 3838.7 | 2420.89 | 4.90[+12] |
| \(A_3\) | 1s\(^2\) 1S\(_0\)–1s3p \(^3\)P\(_1\) | 3838.9 | 3839.5 | 2420.15 | 2.35[+12] |
| \(A_3\) | 1s\(^2\) 1S\(_0\)–1s3p \(^3\)P\(_1\) | 3853.0 | 3854.2 | 2438.08 | 1.63[+12] |
| \(A_3\) | 1s\(^2\) 1S\(_0\)–1s3p \(^3\)P\(_1\) | 3853.9 | 3856.8 | 2440.23 | 5.70[+12] |
| \(A_3\) | 1s\(^2\) 1S\(_0\)–1s3p \(^3\)P\(_1\) | 3854.0 | 3857.1 | 2440.00 | 3.15[+12] |
| \(B_3\) | 1s\(^2\) 1S\(_0\)–1s3p \(^3\)P\(_1\) | 3858.5 | 3859.0 | 2403.89 | 3.32[+12] |
| \(B_3\) | 1s\(^2\) 1S\(_0\)–1s3p \(^3\)P\(_1\) | 3858.7 | 3859.1 | 2403.77 | 6.85[+12] |
| \(B_3\) | 1s\(^2\) 1S\(_0\)–1s3p \(^3\)P\(_1\) | 3859.9 | 3861.2 | 2402.00 | 4.04[+11] |
| \(A_3\) | 1s\(^2\) 1S\(_0\)–1s3p \(^3\)P\(_1\) | 3863.4 | 3865.2 | 2428.63 | 2.79[+13] |
| \(A_3\) | 1s\(^2\) 1S\(_0\)–1s3p \(^3\)P\(_1\) | 3864.1 | 3865.5 | 2430.87 | 6.11[+13] |
| \(A_3\) | 1s\(^2\) 1S\(_0\)–1s3p \(^3\)P\(_1\) | 3866.4 | 3868.2 | 2428.63 | 8.18[+12] |

that ion are also reachable by autoionization. Transitions of the type \(1s^23l–1s3lnl'\) for \(n > 3\) appear on the long-wavelength side of the \(w_3\) line. Blending of these high-\(n\) satellites with the \(y_3\) line may contribute to the underestimate of the \(y_3\) intensity in the collisional–radiative model [28, 29, 60]; however, since the \(1s^23l–1s3l3l'\) feature is so weak, it is unlikely that this is the cause of the remaining discrepancy. There is a phenomenon that is known in the study of configuration interaction where the strength of a class of transitions is transferred to a higher-energy class of transitions when the upper levels of the two classes are interacting [61]. This was seen with the \(2p_{1/2}^56d\) and \(2p_{3/2}^57d\) levels in Ne-like Zr, Nb, Mo and Pd ions; when the \(2p_{1/2}^56d\) and \(2p_{3/2}^57d\) levels crossed, the direction of the strength transfer was reversed [62]. It could be that mixing
between the two $1s^2 3P_1$ levels transfers strength from the (lower-energy) $3P_1$ level to the (higher-energy) $1P_1$ level, thus suppressing the $y_3$ line. There is no way to turn off this mixing in the RELAC calculations.

The corresponding spectrum near $w_4$ ($1s^5 1S_0 - 1s4p 1P_1$) is shown in figure 3, and two groups of satellites are apparent, $A_4$ and $B_4$, with a trace of $C_4$ (also $A_5$), in addition to molybdenum lines [52] at 3621.1 and 3671.0 mÅ. The line at 3649.6 mÅ is of unknown origin. $A_4$ is composed of lines which have upper levels of the form $1s2p4p$ which are populated by dielectronic recombination, while $B_4$ and $C_4$ have upper levels of the form $1s2s4p$ which can either be populated by dielectronic recombination or inner-shell excitation. The transitions contributing to these satellite groups are summarized in table 2. This spectrum was obtained from a chord viewing 8 cm below the midplane ($r/a = 0.3$) in a discharge that had $n_{e0} = 1.6 \times 10^{20} \text{ m}^{-3}$ and $T_{e0} = 1260\text{ eV}$. Also shown in figure 3 is a synthetic spectrum, as described above, with satellite wavelengths from MZ, and the agreement with the observed spectrum is very good.

Moving to higher $n$, the spectrum near $w_5$ ($1s^2 1S_0 - 1s5p 1P_1$) is shown in figure 4, which also includes $w_4$ and the Cl$^{16+}$ Ly$_\beta$ doublet (the individual lines of which are unresolved). The satellite groups $A_5$ and $C_5$ are seen, but $B_5$ is hidden beneath $w_4$. As the $w_n$ series crowds closer together in wavelength, so do the corresponding satellite groups, and $A_6$, $B_6$, $A_7$ and $B_7$ are
Table 2. The calculated Cl$^{15+}$ $n = 4$ resonance and intercombination lines, with Cl$^{14+}$ satellites. The legend is similar to that in table 1.

| Line | Transition       | $\lambda_{MZ}$ (mÅ) | $\lambda_{rel}$ (mÅ) | $g^*f$ | $C_{ex}$ (cm$^3$ s$^{-1}$) |
|------|------------------|----------------------|-----------------------|--------|---------------------------|
| w$_4$ | 1s$^2$ 1S$_0$−1s4p $^1P_1$ | 3603.5 | 3603.3 | 6.436[−2] | 1.422[−13] |
| y$_4$ | 1s$^2$ 1S$_0$−1s4p $^3P_1$ | 3605.3 | 3605.7 | 5.913[−4] | 2.306[−14] |

| $\Delta E_{i,j}$ (eV) | $F_2(i, j)$ (s$^{-1}$) | $C_{IS}$ (cm$^3$ s$^{-1}$) |
|------------------------|------------------------|---------------------------|
| C$_4$                 |                        |                           |
| A$_4$                 |                        |                           |
| B$_4$                 |                        |                           |
| A$_4$                 |                        |                           |
| B$_4$                 |                        |                           |

Table 3. The Cl$^{15+}$ $n = 5$ resonance and intercombination lines, with satellites.

| Line | Transition       | $\lambda_{MZ}$ (mÅ) | $\lambda_{rel}$ (mÅ) | $g^*f$ | $C_{ex}$ (cm$^3$ s$^{-1}$) |
|------|------------------|----------------------|-----------------------|--------|---------------------------|
| w$_5$ | 1s$^2$ 1S$_0$−1s5p $^1P_1$ | 3523.2 | 3523.1 | 3.359[−2] | 6.742[−14] |
| y$_5$ | 1s$^2$ 1S$_0$−1s5p $^3P_1$ | 3524.1 | 3524.6 | 3.042[−4] | 1.070[−14] |

| $\Delta E_{i,j}$ (eV) | $F_2(i, j)$ (s$^{-1}$) | $C_{IS}$ (cm$^3$ s$^{-1}$) |
|------------------------|------------------------|---------------------------|
| C$_5$                 |                        |                           |
| B$_5$                 |                        |                           |
| A$_5$                 |                        |                           |
| B$_5$                 |                        |                           |

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Figure 4. The x-ray spectrum of the Cl$^{15+}$ resonance lines $w_5$ and $w_4$, with satellites, and hydrogen-like Cl$^{16+}$ Ly$_\beta$. The simulated H-, He- and Li-like spectra are shown in purple, green and red, respectively.

also present in this spectrum. Tables 3 and 4 include the relevant information for these lines. The synthetic spectrum using the satellite wavelengths from MZ is shown at the bottom for comparison, again with good agreement. $T_{e0}$ and $n_{e0}$ for the discharge for which this spectrum was obtained were 1260 eV and $1.6 \times 10^{20}$ m$^{-3}$, respectively. Another mystery line, at 3570.4 mÅ, is present.

Finally, the Rydberg series with up to $w_{14}$ resolved is shown in figure 5, for two different times during a 5.4 T, deuterium discharge. In the bottom part is the spectrum from the early portion, when the discharge was limited, with $n_{e0} = 1.4 \times 10^{20}$ m$^{-3}$ and $T_{e0} = 1650$ eV; there are molybdenum lines at 3439.2, 3442.8, 3445.0, 3447.8 and 3450.3 mÅ, respectively, which dominate over $w_8$. The spectrum in the top part is from later in the discharge, with $n_{e0} = 1.6 \times 10^{20}$ m$^{-3}$ and $T_{e0} = 1260$ eV, which also had argon injection, and satellites from $w_3$ in argon [28] (and the next section) cover the chlorine $w_9$, $w_{10}$ and $w_{14}$. The dotted vertical lines show the calculated (RELAC) wavelengths. Between the two spectra, all the lines from $w_7$ to $w_{14}$ are resolved. Two sets of calculated wavelengths, from RELAC and MZ, for the Rydberg series of Cl$^{15+}$ are presented in table 5. The agreement between the two calculations is very good, with the largest differences being of one part in $10^4$, within the experimental uncertainty.
Table 4. The Cl$^{14+}$ satellites for $n = 6 - 10$.

| Line | Transition | $\lambda_{MZ}$ (mÅ) | $\lambda_{rel}$ (mÅ) | $\Delta E_{i,j}$ (eV) | $F_2(i,j)$ (s$^{-1}$) | $C_{IS}$ (cm$^3$s$^{-1}$) |
|------|------------|----------------------|----------------------|----------------------|----------------------|----------------------|
| C$_6$ | 2s $J = \frac{1}{2}-(1s2s6p\,\overline{3}/2)\,\overline{3}/2$ | 3543.9 | 3542.3 | 2691.06 | 1.57[+12] | 6.819[−15] |
| B$_6$ | 2s $J = \frac{1}{2}-(1s2s6p\,\overline{3}/2)\,\overline{3}/2$ | 3563.0 | 3560.7 | 2673.01 | 2.23[+12] | 1.595[−14] |
| A$_6$ | 2p $J = \frac{3}{2}-(1s2p_{1/2}6p_{3/2})\,\overline{3}/2$ | 3574.9 | 3572.1 | 2691.86 | 3.10[+12] | 1.356[−14] |
| A$_6$ | 2p $J = \frac{3}{2}-(1s2p_{3/2}6p_{3/2})\,\overline{5}/2$ | 3575.1 | 3572.2 | 2694.17 | 6.41[+12] | 1.106[−14] |
| A$_6$ | 2p $J = \frac{3}{2}-(1s2p_{3/2}6p_{3/2})\,\overline{5}/2$ | 3575.5 | 3572.6 | 2693.80 | 2.11[+12] | 6.842[−15] |
| B$_7$ | 2s $J = \frac{1}{2}-(1s2s7p\,\overline{3}/2)\,\overline{3}/2$ | 3539.6 | 3537.3 | 2696.08 | 1.75[+12] | 9.507[−15] |
| A$_7$ | 2p $J = \frac{3}{2}-(1s2p_{3/2}7p\,\overline{3}/2)\,\overline{5}/2$ | 3551.8 | 3548.9 | 2717.03 | 3.88[+12] | 6.638[−15] |
| A$_8$ | 2p $J = \frac{3}{2}-(1s2p_{3/2}8p\,\overline{3}/2)\,\overline{5}/2$ | 3563.8 | 3533.9 | 2731.67 | 2.79[+12] | 4.399[−15] |
| A$_9$ | 2p $J = \frac{3}{2}-(1s2p_{3/2}9p\,\overline{3}/2)\,\overline{5}/2$ | 3526.5 | 3523.7 | 2741.85 | 1.93[+12] | 3.015[−15] |
| A$_{10}$ | 2p $J = \frac{3}{2}-(1s2p_{3/2}10p\,\overline{3}/2)\,\overline{5}/2$ | 3519.3 | 3516.5 | 2749.13 | 1.39[+12] | 2.169[−15] |

Table 5. Two calculations of the Cl$^{15+}$ Rydberg series wavelengths, from MZ in the second column and from RELAC in the third column. Measured satellite group wavelengths and measured wavelength differences between the resonance lines and the satellite groups are given in columns four to nine. All wavelengths are in mÅ.

| W$_n$ | C$_n$ | B$_n$ | A$_n$ ($A_3'$) |
|------+------+------|---------------|
| $\lambda_{MZ}$ | $\lambda_{rel}$ | $\lambda_{Exp}$ | $\Delta \lambda$ | $\lambda_{Exp}$ | $\Delta \lambda$ | $\lambda_{Exp}$ | $\Delta \lambda$ |
|——|——|——|——|——|——|——|——|
| 3 | 3789.9 | 3789.6 | 3837.6 | 48.0 | 3858.5 | 68.9 | 3863.9 | 74.3 |
| 4 | 3603.5 | 3603.3 | 3660.0 | 56.7 | 3678.5 | 75.2 | 3690.3 | 87.0 |
| 5 | 3523.2 | 3523.1 | 3583.1 | 60.0 | 3603.5 | (80.4) | 3614.9 | 91.8 |
| 6 | 3481.2 | 3481.2 | 3543.0 | 61.8 | 3562.0 | 80.8 | 3574.7 | 93.5 |
| 7 | 3456.2 | 3456.6 | 3538.6 | 82.0 | 3551.2 | 94.6 |
| 8 | 3440.3 | 3440.7 | (3536.) | (95) |
| 9 | 3429.4 | 3429.8 | 3528.0 | 98.2 |
| 10 | 3421.7 | 3422.1 | 3520.0 | 97.9 |
| 11 | 3416.0 | 3416.4 |
| 12 | 3411.6 | 3412.1 |
| 13 | 3408.3 | 3408.7 |
| 14 | 3405.4 | 3406.1 |

The measured wavelengths of the high-$n$ satellite groups (unresolved) in Cl$^{14+}$ are also summarized in table 5, along with the wavelength differences between the observed satellite
Figure 5. The high-$n$ series of Cl$^{15+}$ with $n$ between 7 and 14. The top spectrum includes some argon lines which obscure the transitions with $n = 9$, 10 and 14, while the bottom spectrum contains several molybdenum lines which dominate the $n = 8$ transition. The vertical dotted lines indicate the calculated wavelengths.

groups of a given $n$ number and the corresponding resonance line calculated from RELAC. The theoretical wavelengths (RELAC) for the resonance lines for the Cl$^{15+}$ Rydberg series have been used for the wavelength calibration. The measured wavelength differences between the resonance lines, $w_n$, and the satellite groups $A_n$, $B_n$ and $C_n$, as a function of $n$ are shown in figure 6. The curves are the theoretical values, from the calculated wavelengths of tables 1–5; the full curves represent the wavelengths from MZ, while the chain curves use the wavelengths from RELAC. These values are taken from the centroids of the calculated satellite groups, as shown in the synthetic spectra. Overall the agreement between theory and experiment is very good, although there is a systematic shift of about 3 mÅ for the $A_n$ lines calculated from RELAC. This offset is possibly due to the configuration interaction in RELAC described above between the $1s2pnp$ and the $1s2sns$ and $1s2snd$ levels which raises the energy of the upper levels in the $A_n$ transitions. The configuration interaction between the $1s2sp4p$ and $1s2p4s$ levels and between the $1s2s5p$ and $1s2p5s$ levels causes the bumps in the $C_n$ and $B_n$ curves at $n = 4$ and 5, respectively.

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Figure 6. The difference between the satellite group wavelengths and the resonance line wavelengths in Cl$^{15+}$ as a function of $n$, for the three satellite groups. The measured values for $A_n$, $B_n$ and $C_n$ are depicted as red asterisks, green triangles and purple dots, respectively. The satellite group $A'_3$ is shown as the orange $\times$. The theoretical wavelength differences are shown by the appropriately coloured curves, with the calculated value for $A'_3$ (from RELAC) given by the orange dot. The full curves are from MZ, while the chain curves are from RELAC. The largest error bars are shown.

4. Argon observations and code comparison

The corresponding high-$n$ transitions and satellites have also been observed in argon. Because argon is a recycling gas, it remains in the plasma for a much longer duration than the chlorine, which allows for weaker lines to be studied. Shown in figure 7 is a spectrum from argon including $w_4$, $w_5$ and $w_6$ from Ar$^{16+}$, $Ly_\beta$ from Ar$^{17+}$ and the satellite groups $A_5$–$A_{12}$, $B_5$–$B_8$ and $C_5$–$C_7$. Plasma parameters for the discharge from which this spectrum was obtained were $n_{e0} = 1.3 \times 10^{20} \text{ m}^{-3}$ and $T_{e0} = 1550 \text{ eV}$. A synthetic spectrum using the calculated satellite wavelengths from MZ is shown in the bottom part, and the agreement is quite good. The transition designations, calculated wavelengths, satellite capture energies, oscillator strengths/satellite
Figure 7. The linear scale x-ray spectrum of helium-like Ar\(^{16+}\) \(w_4\), \(w_5\) and \(w_6\), with satellites, and hydrogen-like Ar\(^{17+}\) Ly\(\beta\), is shown in the top part. In the bottom part is the log-scale observed spectrum (black) and the computed spectrum for Ar\(^{16+}\) (green), Ar\(^{17+}\) (purple) and Ar\(^{15+}\) (red).

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Table 6. The Ar\textsuperscript{16+} n = 4 resonance and intercombination lines, with satellites. The transition designations, wavelengths, satellite capture energies, oscillator strengths/satellite intensity factors and inner-shell excitation rates (at 2000 eV) are given for the strongest lines. The legend is similar to that in table 1.

| Line | Transition | $\lambda_{MZ}$ (mÅ) | $\lambda_{rel}$ (mÅ) | $g^*f$ | $C_{ex}$ (cm\textsuperscript{3} s\textsuperscript{-1}) |
|------|------------|---------------------|---------------------|--------|------------------|
| w\textsubscript{4} | $1s^2 1S_0$→$1s4p ^1P_1$ | 3199.7 | 3199.6 | 6.364[-2] | 1.659[-13] |
| y\textsubscript{4} | $1s^2 1S_0$→$1s4p ^3P_1$ | 3201.2 | 3201.6 | 8.162[-4] | 2.466[-14] |

| C\textsubscript{4} | $2s J = \frac{1}{2}-(1s2p_1/2^4s)_{3/2}$ | 3245.9 | 3246.6 | 2.900.69 | 2.49[+12] | 1.067[-14] |
| C\textsubscript{4} | $2s J = \frac{1}{2}-(1s2s4p_{3/2})_{3/2}$ | 3246.4 | 3247.4 | 2.899.80 | 2.32[+12] | 2.384[-14] |
| C\textsubscript{4} | $2s J = \frac{1}{2}-(1s2s4p_{1/2})_{1/2}$ | 3247.5 | 3247.4 | 2.899.77 | 2.32[+12] | 1.219[-14] |
| B\textsubscript{4} | $2s J = \frac{1}{2}-(1s2s4p_{3/2})_{1/2}$ | 3262.6 | 3262.9 | 2.881.61 | 3.21[+12] | 3.521[-14] |
| B\textsubscript{4} | $2s J = \frac{1}{2}-(1s2s4p_{3/2})_{3/2}$ | 3262.7 | 3263.0 | 2.881.50 | 6.71[+12] | 6.979[-14] |
| A\textsubscript{4} | $2p J = \frac{1}{2}-(1s2p_3/2^4p_{3/2})_{3/2}$ | 3270.6 | 3268.4 | 2.907.36 | 2.21[+12] | 1.167[-14] |
| A\textsubscript{4} | $2p J = \frac{3}{2}-(1s2p_3/2^4p_{3/2})_{1/2}$ | 3271.0 | 3268.8 | 2.910.37 | 3.39[+12] | 1.613[-14] |
| A\textsubscript{4} | $2p J = \frac{3}{2}-(1s2p_3/2^4p_{3/2})_{5/2}$ | 3272.0 | 3269.9 | 2.909.02 | 2.13[+13] | 3.902[-14] |
| A\textsubscript{4} | $2p J = \frac{1}{2}-(1s2p_{1/2}^4p_{3/2})_{3/2}$ | 3272.3 | 3270.1 | 2.905.45 | 9.86[+12] | 5.520[-14] |
| A\textsubscript{4} | $2p J = \frac{3}{2}-(1s2p_{1/2}^4f_{5/2})_{5/2}$ | 3272.4 | 3270.1 | 2.908.51 | 6.45[+12] | 1.426[-14] |
| A\textsubscript{4} | $2p J = \frac{3}{2}-(1s2p_{3/2}^4p_{3/2})_{3/2}$ | 3273.3 | 3271.1 | 2.907.36 | 8.25[+12] | 2.413[-14] |

Table 7. The Ar\textsuperscript{16+} n = 5 resonance and intercombination lines, with satellites.

| Line | Transition | $\lambda_{MZ}$ (mÅ) | $\lambda_{rel}$ (mÅ) | $g^*f$ | $C_{ex}$ (cm\textsuperscript{3} s\textsuperscript{-1}) |
|------|------------|---------------------|---------------------|--------|------------------|
| w\textsubscript{5} | $1s^2 1S_0$→$1s5p ^1P_1$ | 3128.3 | 3128.1 | 3.307[-2] | 7.344[-14] |
| y\textsubscript{5} | $1s^2 1S_0$→$1s5p ^3P_1$ | 3129.0 | 3129.4 | 4.191[-4] | 1.195[-14] |

| C\textsubscript{5} | $2s J = \frac{1}{2}-(1s2s5p_{1/2})_{1/2}$ | 3178.5 | 3177.2 | 2.984.08 | 1.00[+12] | 4.466[-15] |
| C\textsubscript{5} | $2s J = \frac{1}{2}-(1s2s5p_{3/2})_{3/2}$ | 3178.5 | 3177.3 | 2.984.04 | 3.12[+12] | 1.502[-14] |
| B\textsubscript{5} | $2s J = \frac{3}{2}-(1s2s5p_{3/2})_{1/2}$ | 3194.7 | 3192.8 | 2.965.01 | 1.95[+12] | 1.746[-14] |
| B\textsubscript{5} | $2s J = \frac{1}{2}-(1s2s5p_{3/2})_{3/2}$ | 3194.8 | 3192.9 | 2.964.95 | 3.91[+12] | 3.451[-14] |
| A\textsubscript{5} | $2p J = \frac{3}{2}-(1s2p_{3/2}^5p_{1/2})_{1/2}$ | 3204.4 | 3202.0 | 2.989.00 | 2.36[+12] | 8.214[-15] |
| A\textsubscript{5} | $2p J = \frac{1}{2}-(1s2p_{3/2}^5p_{3/2})_{3/2}$ | 3204.7 | 3202.4 | 2.985.41 | 5.36[+12] | 2.718[-14] |
| A\textsubscript{5} | $2p J = \frac{3}{2}-(1s2p_{3/2}^5p_{3/2})_{5/2}$ | 3204.9 | 3202.5 | 2.988.45 | 1.39[+13] | 2.463[-14] |
| A\textsubscript{5} | $2p J = \frac{3}{2}-(1s2p_{3/2}^5p_{3/2})_{3/2}$ | 3205.4 | 3203.1 | 2.987.74 | 3.52[+12] | 1.297[-14] |
Table 8. The Ar\textsuperscript{16+} \( n = 6 \) resonance and intercombination lines, with satellites.

| Line | Transition | \( \lambda_{MZ} \) (mÅ) | \( \lambda_{rel} \) (mÅ) | \( g^*f \) | \( C_{ex} \) (cm\(^3\) s\(^{-1}\)) |
|------|------------|-----------------|-----------------|--------|-----------------|
| w\textsubscript{6} | 1s\textsuperscript{2} 1\textit{S}_0–1s6p \textsuperscript{1}P\textsubscript{1} | 3090.8 | 3091.1 | 2.086[−2] | 4.035[−14] |
| y\textsubscript{6} | 1s\textsuperscript{2} 1\textit{S}_0–1s6p \textsuperscript{3}P\textsubscript{1} | 3091.2 | 3091.5 | 2.576[−4] | 6.646[−15] |

\( \Delta E_{i,j} \) (eV) | \( f_2(i,j) \) (s\(^{-1}\)) | \( C_{IS} \) (cm\(^3\) s\(^{-1}\))

| C\textsubscript{6} | 2s \( J = \frac{1}{2} \)−(1s2s6p\textsubscript{3}2)\textsubscript{3}2 | 3143.2 | 3142.1 | 3027.76 | 1.92[+12] | 7.969[−15] |
| B\textsubscript{6} | 2s \( J = \frac{1}{2} \)−(1s2s6p\textsubscript{3}2)\textsubscript{1}2 | 3159.3 | 3157.5 | 3008.50 | 1.23[+12] | 9.823[−15] |
| B\textsubscript{6} | 2s \( J = \frac{1}{2} \)−(1s2s6p\textsubscript{3}2)\textsubscript{3}2 | 3159.3 | 3157.5 | 3008.47 | 2.47[+12] | 1.944[−14] |
| A\textsubscript{6} | 2p \( J = \frac{1}{2} \)−(1s2p\textsubscript{1}26p\textsubscript{3}2)\textsubscript{3}2 | 3169.2 | 3167.1 | 3028.62 | 3.18[+12] | 1.620[−14] |
| A\textsubscript{6} | 2p \( J = \frac{1}{2} \)−(1s2p\textsubscript{3}26p\textsubscript{3}2)\textsubscript{1}2 | 3169.3 | 3167.2 | 3031.69 | 1.78[+12] | 4.304[−15] |
| A\textsubscript{6} | 2s \( J = \frac{1}{2} \)−(1s2p\textsubscript{3}26p\textsubscript{3}2)\textsubscript{5}2 | 3169.5 | 3167.2 | 3031.57 | 7.57[+12] | 1.315[−14] |
| A\textsubscript{6} | 2p \( J = \frac{1}{2} \)−(1s2p\textsubscript{3}26p\textsubscript{3}2)\textsubscript{3}2 | 3169.8 | 3167.5 | 3031.19 | 2.10[+12] | 7.882[−15] |
| A\textsubscript{6} | 2p \( J = \frac{1}{2} \)−(1s2p\textsubscript{1}26p\textsubscript{3}2)\textsubscript{3}2 | 3168.2 | 3027.23 | 8.19[+11] | 6.016[−15] |

Table 9. The Ar\textsuperscript{16+} \( n = 7 \) resonance and intercombination lines, with satellites.

| Line | Transition | \( \lambda_{MZ} \) (mÅ) | \( \lambda_{rel} \) (mÅ) | \( g^*f \) | \( C_{ex} \) (cm\(^3\) s\(^{-1}\)) |
|------|------------|-----------------|-----------------|--------|-----------------|
| w\textsubscript{7} | 1s\textsuperscript{2} 1\textit{S}_0–1s7p \textsuperscript{1}P\textsubscript{1} | 3068.6 | 3068.9 | 1.724[−2] | 2.456[−14] |
| y\textsubscript{7} | 1s\textsuperscript{2} 1\textit{S}_0–1s7p \textsuperscript{3}P\textsubscript{1} | 3068.9 | 3069.2 | 2.007[−4] | 4.121[−15] |

\( \Delta E_{i,j} \) (eV) | \( f_2(i,j) \) (s\(^{-1}\)) | \( C_{IS} \) (cm\(^3\) s\(^{-1}\))

| C\textsubscript{7} | 2s \( J = \frac{1}{2} \)−(1s2s7p\textsubscript{3}2)\textsubscript{3}2 | 3122.4 | 3121.3 | 3053.99 | 1.02[+12] | 4.416[−15] |
| B\textsubscript{7} | 2s \( J = \frac{1}{2} \)−(1s2s7p\textsubscript{3}2)\textsubscript{1}2 | 3138.4 | 3136.6 | 3034.65 | 7.97[+11] | 5.860[−15] |
| B\textsubscript{7} | 2s \( J = \frac{1}{2} \)−(1s2s7p\textsubscript{3}2)\textsubscript{3}2 | 3138.4 | 3136.6 | 3034.64 | 1.89[+12] | 1.170[−14] |
| A\textsubscript{7} | 2p \( J = \frac{1}{2} \)−(1s2p\textsubscript{1}27p\textsubscript{3}2)\textsubscript{3}2 | 3148.3 | 3146.2 | 3054.64 | 1.56[+12] | 9.135[−15] |
| A\textsubscript{7} | 2p \( J = \frac{1}{2} \)−(1s2p\textsubscript{3}27p\textsubscript{3}2)\textsubscript{5}2 | 3148.6 | 3146.3 | 3057.56 | 4.57[+12] | 7.856[−15] |
| A\textsubscript{7} | 2p \( J = \frac{3}{2} \)−(1s2p\textsubscript{3}27p\textsubscript{3}2)\textsubscript{3}2 | 3148.8 | 3146.5 | 3057.36 | 1.05[+12] | 4.235[−15] |

resonance line wavelengths. As in the chlorine case, the two calculations for the Rydberg series wavelengths for argon are in excellent agreement.

As demonstrated above, the calculated wavelengths for the helium-like Rydberg series lines from MZ and RELAC are in excellent agreement. The agreement between the observed wavelengths and those calculated for the lithium-like satellite groups B\textsubscript{n} and C\textsubscript{n} by the two methods is also quite good. For the satellite groups A\textsubscript{n}, the observed wavelengths and the MZ calculations are also very good, while those from RELAC are systematically 2–3 mÅ too
Table 10. The Ar$^{15+}$ satellites for $n = 8 – 12$.

| Line  | Transition                | $\lambda_{MZ}$ (mÅ) | $\lambda_{rel}$ (mÅ) | $\Delta E_{i,j}$ (eV) | $F_2(i, j)$ (s$^{-1}$) | $C_{IS}$ (cm$^3$ s$^{-1}$) |
|-------|---------------------------|----------------------|----------------------|------------------------|------------------------|-----------------------------|
| B$_8$ | 2s $J = \frac{1}{2} - (1s2s8p_{3/2})_{3/2}$ | 3125.0              | 3125.7              | 3048.46                | 1.06 [+12]             | 7.884 [-15]                 |
| A$_8$ | 2p $J = \frac{3}{2} - (1s2p_{1/2}8p_{3/2})_{3/2}$ | 3134.9              | 3132.8              | 3071.48                | 9.32 [+11]             | 6.025 [-15]                 |
| A$_8$ | 2p $J = \frac{3}{2} - (1s2p_{3/2}8p_{3/2})_{5/2}$ | 3135.2              | 3133.0              | 3074.38                | 3.25 [+12]             | 5.112 [-15]                 |
| A$_8$ | 2p $J = \frac{3}{2} - (1s2p_{3/2}8p_{3/2})_{3/2}$ | 3135.3              | 3133.1              | 3074.23                | 7.29 [+11]             | 3.129 [-15]                 |
| A$_9$ | 2p $J = \frac{3}{2} - (1s2p_{3/2}9p_{3/2})_{5/2}$ | 3126.1              | 3123.9              | 3085.92                | 2.25 [+12]             | 3.520 [-15]                 |
| A$_{10}$ | 2p $J = \frac{3}{2} - (1s2p_{3/2}10p_{3/2})_{5/2}$ | 3119.6              | 3117.4              | 3094.16                | 1.63 [+12]             | 2.520 [-15]                 |
| A$_{11}$ | 2p $J = \frac{3}{2} - (1s2p_{3/2}11p_{3/2})_{5/2}$ | 3114.8              | 3112.6              | 3100.25                | 1.21 [+12]             | 1.880 [-15]                 |
| A$_{12}$ | 2p $J = \frac{3}{2} - (1s2p_{3/2}12p_{3/2})_{5/2}$ | 3111.2              | 3109.0              | 3104.88                | 9.22 [+11]             | 1.427 [-15]                 |

Figure 8. The difference between the satellite wavelengths and the resonance line wavelengths in Ar$^{16+}$ as a function of $n$, for the three satellite groups, along with the theoretical wavelengths. The legend is the same as in figure 6.
Table 11. Two calculations of the Ar\textsuperscript{16+} Rydberg series wavelengths, measured satellite group wavelengths and measured wavelength differences between the resonance lines and the satellite groups. All wavelengths are in mÅ.

| n  | \(\lambda_{\text{MZ}}\) | \(\lambda_{\text{rel}}\) | \(\lambda_{\text{Exp}}\) | \(\Delta\lambda\) | \(\lambda_{\text{Exp}}\) | \(\Delta\lambda\) | \(\lambda_{\text{Exp}}\) | \(\Delta\lambda\) |
|----|----------------|----------------|----------------|----------|----------------|----------|----------------|----------|
| 3  | 3365.7         | 3365.4         | 3405.7         | 40.3     | 3422.8         | 57.4     | 3427.7         | 62.3     |
| 4  | 3199.7         | 3199.6         | 3246.2         | 46.6     | 3262.3         | 62.7     | 3272.0         | 72.4     |
| 5  | 3128.3         | 3128.1         | 3178.4         | 50.3     | 3194.8         | 66.7     | 3204.4         | 76.3     |
| 6  | 3090.8         | 3091.1         | 3143.6         | 52.5     | 3159.3         | 68.2     | 3169.6         | 78.5     |
| 7  | 3068.6         | 3068.9         | 3122.1         | 53.2     | 3138.6         | 69.7     | 3148.4         | 79.5     |
| 8  | 3054.4         | 3054.8         | 3125.6         | 70.8     | 3135.0         | 80.2     |                |          |
| 9  | 3044.7         | 3045.1         |                |          | 3125.6         | 80.5     |                |          |
| 10 | 3037.8         | 3038.2         |                |          | 3119.4         | 81.2     |                |          |
| 11 | 3032.8         | 3033.1         |                |          | 3115.3         | 82.2     |                |          |
| 12 | 3028.9         | 3029.2         |                |          | 3111.0         | 81.8     |                |          |
| 13 | 3025.9         | 3026.3         |                |          |                |          |                |          |

short. This may be due to residual Coulomb interactions among different terms of a single configuration in the upper levels of the \(A_n\) transitions. A comparison may also be made for the satellite intensity factors calculated via the two approaches. In figure 9 the satellite intensity factors calculated from RELAC and MZ for the satellites of Ar\textsuperscript{15+} are shown. There is excellent agreement for the transitions which contribute to \(A_n\) and \(B_n\), over two orders of magnitude. In general, most of the points are within 20% of each other for the two calculations. The largest deviations are found for the transitions contributing to \(C_n\), and in particular for \(C_3\). However, for the plasma conditions considered here, where the population of the upper levels of \(C_3\) is dominated by inner-shell excitation of lithium-like argon, it is difficult to distinguish between the \(F_2\)'s computed by the two methods.

Spectra of \(w_4\) and satellites for plasmas with different central electron temperatures are shown in figure 10. As the temperature decreases, the intensities of the satellite groups (relative to \(w_4\)) increase; in the bottom part with an electron temperature of less than 1000 eV, the satellite group \(A_4\) is nearly as bright as the resonance line. Similar observations were made from Alcator C [26], from radial profile measurements; in fact, near the plasma periphery, the satellite group \(A_5\) was actually brighter than \(w_5\). Also shown in the figure are the corresponding synthetic spectra, generated as described above (using the MZ wavelengths), which have been normalized to \(w_4\). The relative intensities of the satellites \(A_4\), \(B_4\) and \(C_4\) (and \(A_5\)) are well reproduced for these three different electron temperature plasmas, supporting the dielectronic recombination and inner-shell excitation rates presented in the tables. (A strong molybdenum [52] line at 3230.1 mÅ is visible in these spectra.)

There is evidence for the argon intercombination line \(y_4\) on the long-wavelength side of \(w_4\). In figure 11 the spectrum in the immediate vicinity of \(w_4\) is shown; the observed spectrum is depicted by asterisks. The full green curve centred on 3199.6 mÅ is the calculated resonance line, normalized at the peak, with the appropriate width from the instrumental resolution and Doppler broadening. The green curve centred on 3201.6 mÅ is the intercombination line \(y_4\), with
Figure 9. The $\text{Ar}^{15+}$ satellite intensity factors computed from RELAC (abscissa) and MZ (ordinate). The red asterisks, green triangles, orange crosses and purple circles are for the various transitions contributing to the satellite groups $\text{A}_n$, $\text{B}_n$, $\text{A'}_n$ and $\text{C}_n$, respectively.

the calculated wavelength but with the observed intensity. Shown in purple are two helium-like satellites to $\text{Ar}^{17+}$ Ly$_{\beta}$, 1s2s $^1S_0$–2p3s $^1P_1$ and 1s2p $^1P_1$–2p3p $^1D_2$, with calculated wavelengths of 3197.7 and 3206.6 mÅ, respectively. (The former decay is enabled by configuration interaction between the 2p3s $^1P_1$ level and the 2s3p $^3P_1$ and 2s3p $^1P_1$ levels (the calculation of the interaction is actually carried out in intermediate coupling on $jj$-coupled basis functions). In the collisional–radiative model, at $T_e = 2$ keV these lines are excited more than 99% by dielectronic recombination from the ground level of the hydrogen-like ion.) The full black curve is the composite calculated spectrum, which agrees well with the data points. Without inclusion of the theoretical $\gamma_4$ line, there would be excess emission around 3202 mÅ. The actual best-fit experimental wavelength for $\gamma_4$ is 3201.3 mÅ, which agrees well with the calculation. The calculated ratio of $\gamma_4/\omega_4$ for these discharge conditions (2050 eV and $1.1 \times 10^{20}$ m$^{-3}$) is 0.029, whereas the observed ratio is around 0.05 in figure 11. This may be related to the ratio $\gamma_3/\omega_3$ observed to be a factor of two higher than predicted [28].

Spectra near the $\text{Ar}^{16+}$ Rydberg series limit [26] are shown in figure 12. The top spectrum was taken along the central chord of a plasma with $n_{e0} = 0.9 \times 10^{20}$ m$^{-3}$ and $T_{e0} = 2600$ eV. The
Figure 10. The observed x-ray spectra of Ar\textsuperscript{16+} \textit{w}\textsubscript{4} with satellites, for three different central electron temperatures, are shown in black. The calculated spectra for \textit{w}\textsubscript{4}, \textit{A}\textsubscript{4} and \textit{A}\textsubscript{5} are shown in red, \textit{C}\textsubscript{4} in purple and \textit{B}\textsubscript{4} in green.

resonance lines from \textit{w}\textsubscript{6} to \textit{w}\textsubscript{14} are clearly resolved, and there is a region of enhanced brightness from \textit{w}\textsubscript{10} up to the series limit at 3008.8 mÅ, presumably due to unresolved lines. Along this chord, most of the line emission is from the plasma centre where electron impact excitation is the dominant mechanism for populating the upper levels. The continuum at wavelengths shorter than the limit is greater than the continuum level between the resonance lines, and is due to radiative recombination [26]. Ar\textsuperscript{17+} \textsc{Ly}\textsubscript{γ} near 2987.4 mÅ is also prominent. The corresponding spectrum from an identical plasma, but taken along a chord viewing through \(r/a = 0.67\), where the electron temperature was 1100 eV and the electron density was \(0.8 \times 10^{20} \text{ m}^{-3}\), is shown in the middle part of figure 12. The lines are greatly reduced in intensity and the widths are very narrow due to the lower ion temperature. The intensities of \textit{w}\textsubscript{9} and \textit{w}\textsubscript{10} are enhanced relative to the trend of decreasing intensity with increasing \(n\) number, which is due to population by charge-exchange recombination with intrinsic neutral deuterium in the ground state, near the plasma edge [26, 63]. Emission from the very high \(n\) levels (\(n > 25\)) is also visible just on the long-wavelength side of series limit. Along this chord, however, the lines \textit{w}\textsubscript{11} through \textit{w}\textsubscript{14} are not visible. The viewing chord of the middle spectrum was 18.5 cm above the midplane in a discharge with a lower X-point. The spectrum shown in the bottom part is from a somewhat similar plasma, from a chord viewing through \(r/a = 0.62\), but 19.7 cm below the midplane, for a lower X-point discharge. In this case
$w_{10}$ is enhanced relative to the other $w_n$ lines (due to population by charge exchange with intrinsic neutral deuterium in the ground state) and the feature on the long-wavelength side of the limit is now dominant. This feature is from $n$ numbers between 30 and 40, and is due to charge exchange between hydrogen-like argon and intrinsic neutral deuterium in the $n = 3$ and 4 excited states [26,63]. The reason that this feature is so prominent in the bottom of the plasma near the X-point is because the neutral density is concentrated there [48,57]. Why there is no feature from $n \sim 20$ at 3018 mA, which would be from charge-exchange $n = 2$ excited deuterium, is unknown. In this spectrum, $w_{12}$ through $w_{14}$ are again absent. Why $w_{11}$ is visible here but not in the spectrum from above the midplane is not clear, but may be related to the fact that $w_{10}$ is strong here, and $w_9$ was dominant in the middle spectrum. (The bottom spectrum was obtained from a different plasma on a different day from a different spectrometer.)
19.23

Figure 12. Spectra near the Ar$^{16+}$ series limit. In the top part is the spectrum from a central chord view, in the middle part is a spectrum from an identical plasma with a view 18.5 cm above the midplane ($r/a = 0.67$) and in the bottom part is a spectrum from a similar plasma with a view 19.7 cm below the midplane ($r/a = 0.62$). The ionization limit is shown as the vertical line. The lower spectrum was cut off below 2990 mÅ.

5. Sulfur observations and code comparison

Finally, the Rydberg series of helium-like S$^{14+}$ from $w_5$ to $w_{13}$ is shown in figure 13, which was obtained from a plasma with $n_{e0} = 2.0 \times 10^{20} \text{ m}^{-3}$ and $T_{e0} = 1100 \text{ eV}$. Unlike the cases of argon and chlorine, for sulfur the hydrogen-like Ly$\beta$ doublet is on the short-wavelength side of $w_5$. Also apparent is a molybdenum line at 3834.8 mÅ [52], in addition to $A_3$ in Cl$^{14+}$. The wavelengths and oscillator strengths for the helium-like lines calculated by RELAC and MZ are presented in table 12, again with the wavelengths in excellent agreement. The simulated spectrum is also shown in figure 13. The strongest components of the satellite groups $A_n$ are the transitions of the form $1s^22pJ = \frac{3}{2}-(1s2p_{3/2}np3/2)_{5/2} (1s^22p^2P_{3/2} - 1s2p^{(3)}P_{n} 2D_{5/2} \text{ in } LS$-coupling notation). The wavelengths and satellite intensity factors for these transitions calculated from MZ and RELAC with $3 \leq n \leq 10$ for S$^{13+}$ are presented in table 13. Similar to the cases for chlorine and argon, the RELAC wavelengths are $\sim 3.5$ mÅ longer, while the $F_2$ values are in excellent agreement. The sulfur levels in Alcator C-Mod are too low for these satellites to be measured.

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Figure 13. The Rydberg series of helium-like $S^{14+}$ for $n \geq 5$. In green (purple) is the simulated spectrum for $S^{14+}$ ($S^{15+}$).

Table 12. Two calculations of the $S^{14+}$ Rydberg series wavelengths (in mÅ), along with radiative transition probabilities ($s^{-1}$) and oscillator strengths.

| $n$ | $\lambda_{MZ}$ (mÅ) | $\lambda_{rel}$ (mÅ) | $A_{ij}$ ($s^{-1}$) | $g^* f$ |
|-----|-----------------------|----------------------|---------------------|---------|
| 3   | 4088.5                | 4088.9               | 7.28[12]            | 0.0637  |
| 4   | 3997.7                | 3998.2               | 3.63[12]            | 0.0324  |
| 5   | 3950.1                | 3950.5               | 2.07[12]            | 0.0192  |
| 6   | 3921.9                | 3922.4               | 1.29[12]            | 0.0126  |
| 7   | 3903.8                | 3904.3               | 8.60[11]            | 0.0090  |
| 8   | 3891.5                | 3892.0               | 6.02[11]            | 0.0069  |
| 9   | 3882.8                | 3883.3               | 4.38[11]            | 0.0056  |
| 10  | 3876.3                | 3876.8               | 3.28[11]            | 0.0049  |
| 11  | 3871.5                | 3871.9               | 2.52[11]            | 0.0050  |
| 12  | 3867.7                | 3868.1               | 1.98[11]            | 0.0074  |

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Table 13. Two calculations of the strongest components of the $A_n$ series in $S^{13+}, 1s^22p \ J = \frac{3}{2} - (1s2p_{3/2}n3/2)_{5/2}$. Wavelengths are given in the second and third columns, satellite intensity factors are presented in the fourth and fifth columns, capture energies from RELAC are shown in the sixth column and in the last column are inner-shell excitation rates (at 1500 eV) from RELAC.

| $n$ | $\lambda_{MZ}$ (mÅ) | $\lambda_{rel}$ (mÅ) | $F_{2,MZ}$ (s$^{-1}$) | $F_{2,Rel}$ (s$^{-1}$) | $\Delta E_{i,j}$ (eV) | $C_{IS}$ (cm$^3$ s$^{-1}$) |
|-----|----------------|----------------|----------------|----------------|----------------|----------------|
| 3   | 4388.6         | 4386.5         | 5.52 [+13]     | 5.21 [+13]     | 2149.50        | 7.867 [-14]    |
| 4   | 4193.0         | 4189.0         | 1.82 [+13]     | 1.72 [+13]     | 2282.78        | 1.699 [-14]    |
| 5   | 4108.1         | 4104.4         | 1.03 [+13]     | 1.04 [+13]     | 2343.79        | 9.056 [-15]    |
| 6   | 4063.6         | 4060.0         | 6.02 [+12]     | 5.87 [+12]     | 2376.79        | 4.750 [-15]    |
| 7   | 4037.3         | 4033.7         | 3.66 [+12]     | 3.58 [+12]     | 2396.73        | 2.895 [-15]    |
| 8   | 4020.4         | 4016.8         | 2.39 [+12]     | 2.34 [+12]     | 2409.62        | 1.924 [-15]    |
| 9   | 4008.9         | 4005.4         | 1.65 [+12]     | 1.62 [+12]     | 2418.45        | 1.315 [-15]    |
| 10  | 4000.7         | 3997.2         | 1.19 [+12]     | 1.16 [+12]     | 2424.77        | 9.402 [-16]    |

6. Conclusions

The high-$n$ Rydberg series of helium-like Cl, Ar and S have been observed from Alcator C-Mod plasmas. The associated lithium-like satellites up to $n = 12$ for Cl and Ar have also been seen. Comparison of observed satellite wavelengths has been made with calculations from two different atomic structure codes, RELAC and MZ, and there is good agreement in general, although the $A_n$s from RELAC, with lower levels of the form $1s^22p$, differ by 2–3 mÅ. Calculated wavelengths for the helium-like resonance lines, $w_n$, from the two different methods are in excellent agreement. The calculated intensities of the satellite groups relative to the resonance lines are also in good agreement with the observed line brightnesses, verifying the dielectronic recombination and inner-shell excitation rates. A large majority of the satellite intensity factors, $F_2$, computed by the two approaches, is within 20%. The intercombination line $\gamma_4$ has been observed for argon.

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