Published in final edited form as:

Eur J Phys. 2018 ; 72: . doi:10.1140/epjd/e2018-90118-7.

Analysis of EUV spectra from N-shell tungsten ions observed with an electron beam ion trap

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Abstract

Extreme ultraviolet spectra of highly charged tungsten ions were produced with an electron beam ion trap at the National Institute of Standards and Technology and recorded with a flat-field grazing-incidence spectrometer. The spectra were measured in the wavelength range 2.7–17.3 nm while the beam energy varied between 1.65 and 2.00 keV. At these energies, the ionization stages from Zr-like W³⁴⁺ to Se-like W⁴⁰⁺ ions were observed. Large-scale collisional-radiative modelling was used to identify the strong lines, including 15 new ones, which represent electric dipole $n = 4-4$ transitions in these ions. While a good quantitative agreement between theoretical and experimental data was found for almost all ions, some of the tentatively identified wavelengths in W³⁵⁺ significantly disagree from all available calculations.

1 Introduction

Due to its high melting point and low erosion characteristics [1,2], tungsten has received a great deal of attention for applications in magnetic confinement fusion. It is expected to be a plasma facing material in the divertor region of the fusion reactor ITER, currently under construction in Cadarache, France. The sputtering caused by energetic plasma particles will result in tungsten ions penetrating different parts of the plasma volume with temperatures from several eV to about 20 keV. Tungsten has atomic number $Z = 74$, and because of this large number of electrons, ions of different charges will be present in the reactor. The plasma emission spectra will therefore contain many lines coming from a number of ionization stages of tungsten. These spectral lines and their intensity ratios can be used to derive different plasma parameters, such as electron density, temperature, and ion density. Even more importantly, the emission spectra of tungsten will result in strong radiative power losses that are to be carefully controlled in order to assure a sustainable operation mode of a fusion reactor.

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Author contribution statement

The experiment was conceived and performed by Y.A.P., J.D.G., and Y.R. The theoretical calculations were performed by T.D. and Y.R. The analysis and identifications of the spectra were performed by T.D., J.R., and Y.R. All authors contributed to manuscript preparation.

The intermediate charge states of tungsten from Zr-like W^{34+} to Se-like W^{40+} are expected to be present in the fusion plasma with electron temperatures on the order of several hundred electronvolts. A number of papers on the X-ray and extreme ultraviolet (EUV) spectra from these ionization stages have appeared in the literature [3–14] with electron beam ion traps (EBITs) being the primary tool for spectra production and analysis. For instance, in one of the first EBIT works on tungsten, Radtke et al. [5] used an EBIT equipped with a 2-m grazing-incidence spectrometer to record spectra of I-like W^{21+} to Cu-like W^{45+} in the spectral range of 4.5–7.0 nm. The beam energies in this experiment varied from 500 eV to 4 keV. A collisional-radiative (CR) model with an assumed electron density of 10^{12} cm^{-3} that is in the typical range for EBIT conditions was used to analyze the observed spectra. Later, the same group measured EUV emission in In-like W^{25+} to Sr-like W^{36+} in the 5.0–5.4 nm region at electron beam energies between 0.9 and 1.7 keV [6], and the measured spectra were also compared with the theoretical results obtained from a CR calculation. An important paper on the analysis of W emission was published by Utter et al. [7] who recorded spectra of Rb-like W^{37+} to Cu-like W^{45+} between 4.0 and 8.5 nm with a flat-field spectrometer having a variable line spaced grating of 2400 grooves/mm. In order to deduce the wavelengths and line intensity ratios, they calculated spectra based on the wavelength predictions of Fournier [15]. More recently, Ralchenko et al. [10] measured spectra of Br-like W^{39+} to Co-like W^{47+} on the NIST EBIT and analyzed them using a CR code NOMAD [16]. These and other spectroscopic data for various ions of tungsten were compiled in reference [17] and are available in the NIST Atomic Spectra Database [18].

The present work addresses several objectives. First, spectra from complex ions with an open N shell offer a very demanding benchmark for CR codes. The number of excited states from the N-shell ions that are to be taken into account in CR modeling increase immensely with the addition of electrons to the $4d$ subshell. Therefore, any attempt to simulate spectra from $4d^N$ ions becomes an extremely challenging computational task. To this end, newly measured highly-quality spectra provide invaluable benchmark data for CR models.

2 Experiment

The measurements were performed at the EBIT facility at NIST [19,20]. The highly-charged ions are produced with an energetic electron beam (typical electron density on the order of $n_e \approx 10^{11} \text{ cm}^{-3}$ to 10^{12} cm^{-3}) and are contained in a radial trap created by the Coulomb field of the beam and a superconducting 2.8 T magnet, and axially by two drift tubes at 500 V and 220 V potentials, with the asymmetry being used to prevent the escape of ions towards the electron gun. Due to the fine control of the electron beam energy, the element of study can be ionized to a selected ionization stage. In the present experiment, the electron beam energy was varied between 1.65 and 2.00 keV with the beam currents ranging between 52.3 and 61.8 mA.

Tungsten was injected into the trap by a multi-cathode Metal Vapor Vacuum Arc (MeVVA) [21]. The trap was emptied every 10 s to prevent the build-up of contaminants. The EUV spectra were recorded with a flat-field grazing-incidence spectrometer [22] equipped with a variable line-space grating. The liquid-nitrogen-cooled charge coupled device (CCD) had a matrix of 2048 pixels $\times$ 512 pixels (pixel size $13.5 \mu\text{m} \times 13.5 \mu\text{m}$). Measured spectra

consisted of 10 exposures, each 60 s in duration. To correct for spurious signals created by cosmic rays, a filtering program was used to automatically remove data points lying outside of five standard deviations of the true signals in each pixel.

The elements used for wavelength calibration were injected via a gas-injection system [23] or are present intrinsically in the EBIT. The wavelength calibration was performed using about 20 well-known lines of oxygen (O^{4+} and O^{5+}), neon (Ne^{4+} , Ne^{5+} , Ne^{6+} , and Ne^{7+}), xenon (Xe^{42+} and Xe^{43+}), and barium (Ba^{45+}). The gases (Xe, Ne and CO_2) were injected into the trap while Ba is a naturally occurring impurity in the EBIT [24]. Data were taken for neon at 2 and 4 keV, and for CO_2 at 2 keV. The spectrum of Ba was taken as a background spectrum at 5.8 keV. Calibration lines were fit with unweighted Gaussian profiles. A third-order polynomial was calculated to relate wavelengths to detector channels. The uncertainty of finding the peak for each line profile was added in quadrature with an estimated systematic wavelength uncertainty to obtain a final uncertainty for each measured wavelength. The systematic uncertainty was found by requiring $\chi^2 = n - N$, where n is the number of calibration values and N is the number of degrees of freedom [25]. This estimate of systematic uncertainty was found to be 0.00055 nm.

3 Collisional-radiative modelling

The analysis of the observed tungsten spectra was based on the results of steady-state CR modeling of the EBIT plasma. The CR simulations were performed with the non-Maxwellian CR code NOMAD [26], using atomic radiative and collisional data calculated with the Flexible Atomic Code (FAC) [27]. A detailed description of our approach to CR modeling of non-Maxwellian EBIT plasmas can be found in, e.g., [28], therefore below we only provide a short description as well as point out some important issues relevant to the present study.

The starting point for construction of any CR model is an appropriate description of the atomic structure of the ions involved as well as selection of a proper method for calculation of atomic data. The use of the FAC for tungsten ions with charges on the order of 30–45 is well justified since it is based on a fully-relativistic model potential method including quantum-electrodynamic effects and has consistently shown a good accuracy for highly-charged ions (e.g., [10]). Since our EUV spectrometer provides an adequate resolution of the order of $\lambda/\delta\lambda \approx 350$, the model had to be built in terms of the atomic fine-structure levels. The actual calculation of atomic data was performed in two steps. First, for each ion the energy levels, radiative transition rates (up to electric and magnetic quadrupoles), and collisional excitation, ionization and radiative recombination cross sections are calculated for the ground configuration, singly-excited configurations (up to a maximal principal quantum number $n_{\max}$ depending on the complexity of an ion), and configurations arising from double excitations within the $n = 4$ shell. These levels that are noticeably populated under the low-density EBIT conditions and thus are to be accounted for in the CR model. For instance, single excitations from the $4f$ /subshells included transitions within the $n = 4$ complex of Tc-like W^{31+} to Y-like W^{35+} ions and within $n = 4, 5$ and 6 complexes of Sr-like W^{36+} to As-like W^{41+} ions. The double excitations contained the transitions within the $n = 4$ shell of Rb-like W^{37+} to As-like W^{41+} ions. Although this approach is sufficiently accurate

for many applications, it should however be refined for our spectroscopic measurements. Therefore, as a second step, we recalculated the energies of the lowest $n = 4$ levels by including all possible excitations (up to double, triple or quadrupole excitation depending on the complexity of the ions) within the $n = 4$ complex. It was repeatedly shown in our previous papers (see, e.g., [28,29] and references therein) that accounting for multiple excitations within the ground configuration complex improves agreement with the experiment. Accordingly, the energies of the singly and doubly-excited configurations included in the CR model were updated by the new energies from the second run.

The CR model altogether included data for 11 ion stages, from Tc-like W^{31+} to As-like W^{41+} , and a total of 38 595 energy levels. Since ions far from the maximum abundance are populated very little and thus do not contribute to the observed spectra, a typical simulation included only 6–7 ionization stages. The steady-state ionization balance, ion and level populations, and synthetic spectra were calculated assuming a Gaussian electron energy distribution function for the EBIT beam with the electron density $n_e = 10^{11} \text{ cm}^{-3}$. The steady-state approximation was justified by time-dependent calculations that showed that it is reached within a fraction of a second, while the trap was emptied and refilled after every 10 s. The electron beam energy used in simulations was corrected for the space charge that may be as high as 250 eV depending on the amount of neutralization by the trapped ions. Note that the experimental (nominal) beam energy is given below without any corrections and therefore it is typically larger than the theoretical energy. The free parameter in our simulations was the rate of charge exchange between the ions and the neutral atoms that are present in the trap. Finally, the theoretical spectra were convolved with the spectrometer efficiency curve shown by the dashed blue line in Figure 1b and compared with the measured spectra.

4 Line identifications

Figures 1a–1c show the measured spectra in the wavelength range from 2.7 to 17.3 nm for eight electron beam energies from 1.65 to 2.00 keV. The intensity values are given in analog-to-digital units (ADU) of the CCD detector. The predicted second (third) order spectrum that was obtained by doubling (tripling) the wavelength of the measured spectrum is shown in red (green) as a vertically shifted line. One can clearly see that a number of lines above 9 nm are due to the higher order spectra.

The identifications of the 41 measured lines (15 are new lines) are listed in Table 1. The upper and lower levels for each transition are given along with the calculated transition probabilities and the previously measured and/or theoretical values. FAC calculations were performed in the intermediate coupling; however, as customary for such highly charged ions, the level designations are given in the jj-coupling using the largest component in the corresponding wavefunction. We use standard notation for electron angular momenta so that $n l \pm$ corresponds to the total angular momentum $j = l \pm 1/2$ of an electron with the principal quantum number n . As seen in Table 1, nearly all identified lines represent electric dipole transitions (E1) into the ground state $4d^k$ or $4p^k$ from different $n = 4$ excited states.

Since our wavelength range partially overlaps with the previous EBIT measurements of reference [7], a number of the presently measured lines are already known and are accordingly marked in the table. The agreement between the two independent EBIT measurements, as will be also discussed below, is generally very good. In reference [7] the wavelengths and intensities of their observed spectra are based on calculations by Fournier [15]; these transition wavelengths were obtained with the relativistic RELAC code using a similar relativistic model-potential method implemented in FAC. However, only singly excited configurations (up to $n = 5$ only) were included in reference [15] which explains a generally larger disagreement between RELAC results and the experimental wavelengths compared with the present work. Another method that has recently applied to calculations of energy levels and spectral line wavelengths and transition probabilities in highly-charged ions relevant to this work is the ab initio quasirelativistic Hartree-Fock method (QRHF) [30–33]. This technique, which is based on frozen-core approximation and variational determination of transformed radial orbitals with account of configuration interaction, provides good description of energy structure and spectra for highly-charged ions.

Two typical examples of comparisons between simulations and measurements for the short wavelengths are given in Figures 2a and 2b. As mentioned above, the longer-wavelength emission is mostly due to high-order spectra and therefore we restrict this demonstration to the range of 4–9 nm. In Figure 2a the observed spectrum at 1.90 keV is presented along with the best matching calculated spectrum at the beam energy of 1.68 keV. The energy difference is due to effects of the space charge in the trap, which is known to lower the effective energy of the incoming electrons. The strongest lines in the modeled spectrum are due to Y-like, Sr-like, and Rb-like ions of W with ionization energies (IE) of 1.5124, 1.5691, and 1.6217 keV, respectively [18]. Figure 2b compares the observed spectrum at 1.95 keV with the calculated spectrum at 1.79 keV where most of the lines are due to Rb-like, Kr-like (IE = 1.8298 keV) and Br-like (IE = 1.8829 keV) ions. These comparisons clearly reveal a quite reasonable agreement between the measured and calculated relative intensities which is the most important factor in line identification. The relative intensities of the measured spectra as well as those of the modelled spectra are also given in Table 1. Here, the intensities of all the lines are normalized to that of the strongest observed transition. Deviations from the predicted ratios in many cases can be attributed to overlaps with other lines.

4.1 W XXXV

The ionization energy of the lowest measured ion, Zr-like W^{34+} , is 1459.9 eV [18] and therefore it can be produced with the low electron beam energies of the present experiment. With the ground configuration of $4s^2 4p^6 4d^4$ the number of possible states are very large even for the single $n = 0$ excitations, and thus this ion is extremely challenging to model reliably. Due to computational limitations, in the present FAC calculations for W^{34+} we included only single excitations within the $n = 4$ complex and single excitations of $4d$ electrons into the $n = 5$ complex and into the $6s$ and $6p$ states. Even this rather limited calculation generated about 4100 energy levels with more than 1 500 000 spectral lines within the experimental spectral range. However, the modeled spectrum shows only one strong electric-dipole resonance line $(4d-4)_0 - ((4d-3)_{3,2}, 4f-)_{1,1}$ with a wavelength of (5.1097

± 0.0009) nm that was newly identified. Since the upper level of this transition is strongly connected with the ground level $(4d^{-4})_0$, it is almost exclusively populated by the electron-impact excitation from the latter. Very recently, Karpuškien et al. [33] used QRHF to calculate energy levels for the first three configurations of W^{34+} as well as the wavelengths and transition probabilities. Since no wavelengths are provided in [33], it is necessary to find correspondence between their energy levels with notations in LS-coupling with our FAC results to derive the Ritz wavelengths. For instance, we identified their level with the sequential number 189 with our level 202 as both have the same angular momentum $J=1^-$ and both are number 19 in the list of all $J=1$ levels of negative parity. The corresponding wavelength from reference [33] is thus 5.240 nm which is about 2.5% higher than the measured value. Note that the transition probability of $1.79 \times 10^{12} \text{ s}^{-1}$ is reasonably close to our value of $2.81 \times 10^{12} \text{ s}^{-1}$ which is an additional confirmation of correct match of the levels.

4.2 W XXXVI

The Y-like W^{35+} (Fig. 1a) turned out to be the most problematic ion in this study. With the three electrons in the $4d$ shell of the ground state, it produces a very large number of excited states: our CR model with single and double excitations (for $n=4$ only) includes more than 2400 levels. The calculated spectrum shows three strong lines that are *tentatively* identified in the experiment. The presence of those three lines was already clear in the theoretical spectra of Figure 4 in [6] although no identifications were provided. Our identification of these lines is primarily based on their intensity variation with the electron beam energy. The disagreement between calculated and measured wavelengths is significant and reaches 0.421 and 0.063 nm for lines marked Y1 and Y3, respectively, in Table 1; therefore, these lines are marked with “T” (tentative). Such a substantial difference in wavelength for Y1 is uncommon in our calculations that generally agree with EUV measurements within 0.1 nm.

The level energies for low-excited configurations of Y-like ion were recently calculated in reference [32] using QRHM. Their wavelengths for the three transitions are also given in Table 1, and one can clearly see that the agreement with the measured wavelengths is marginal, too. This discrepancy calls for additional theoretical and experimental analysis of the spectra from W^{35+} . It is also interesting to note that the theory and the experiment agree quite well for the neighboring Zr-like and Sr-like ions.

4.3 W XXXVII

The Sr-like ion W^{36+} (Fig. 1b, lower panel) has the ground configuration of $4s^2 4p^6 4d^2$. The total number of included atomic levels in our CR model for this ion is almost 5000. As was mentioned above, the energies of the lowest levels in the model were corrected using a much larger atomic structure calculation. In case of the Sr-like ion, this calculation included only triple excitations within $n=4$ and yet the total number of fine structure levels was more than 200 000.

We identified six new spectral lines that are best resolved at the electron beam energy of 1.87 keV. All lines correspond to $4p-4d$ and $4d-4fE1$ transitions. The identifications for three of these lines, namely, marked Sr3 (5.5652 nm), Sr5 (6.5711 nm) and Sr6 (6.7168 nm),

are tentative because of significant blends. However, the agreements between calculated and measured wavelengths are very good, typically within 0.5%. The QRHM results of [31] also agree very well with our calculations.

4.4 W XXXVIII

The Rb-like W^{37+} is a quasi-one-electron system with the ground configuration $4s^2 4p^6 4d$. Our CR model included all possible singly-excited configurations up to $n = 6$ complex and all possible doubly and triply excited configurations in the $n = 4$ complexes, bringing the total number of levels to more than 7100. We identified 14 lines, given in Table 1 and indicated in Figure 1c at 1.90 keV electron beam energy. Five of these lines are new; the other nine were previously reported in reference [7]. The measured wavelengths are in good agreement with theory, however, not all the identifications are clearly matched. As shown in Table 1, the line at 6.1901 nm, Rb4, is a blend of two calculated lines. In reference [7] this line is also listed as a blend of two calculated transitions, of which the first agrees with our identification, while the second corresponds to a different calculated transition. The line keyed as Rb6 at 6.3428 nm is identified as a blend of three calculated transitions. The close line Rb4 at 6.34319 nm in [7] is given as a blend of two calculated transitions, neither of which corresponds to our present identifications. The line Rb10 at 8.0142 nm is new and identified as a blend of two transitions. Finally, the line Rb12 at 8.1877 nm is also associated with a blend of two transitions which agrees with reference [7].

The QRHF calculations [30] agree with our identifications of the upper and lower levels for all transitions in the table. However, their calculated wavelengths, on the average, show worse agreement with the measured wavelengths. Kilbane [13] also performed calculations for this charge state with FAC but using only singly-excited states. Therefore their calculated wavelengths are not very close to the experimental data, and hence we do not show them in the table.

4.5 W XXXIX

The three lines from Kr-like W^{38+} identified in our measured spectra (see Fig. 1c) have already been observed by Utter et al. [7] with smaller uncertainties. However, their identifications for two longer-wavelength lines are different both from the original calculations of [15] that were the basis of their analysis and from the present calculations that agree with the RELAC results. Therefore, it seems that the misidentification of the two lowest levels in [7] might be the result of misprints.

The measured lines correspond to the electric-dipole transitions into the ground state $4s^2 4p^6 \ ^1S_0$ and thus the upper levels all have $J = 1$. The possible excitations from the closed-shell ground state result in fewer possible combinations of angular momenta and thus in fewer excited states than for other ions of W. Nonetheless, our CR model for W^{38+} is rather extensive and includes 1241 levels. The level energies were calculated including up to quadruple excitations within the $n = 4$ complex and single excitations into higher shells. This may explain the fact that our theoretical wavelengths are generally closer to the measured values than those of [15].

Finally note that Utter et al. [7] also reported four unknown lines from Kr-like W between 4.9 and 6.3 nm. Neither our measurements nor our simulated spectra confirm the presence of these lines.

4.6 W XL

The spectral lines from Br-like ion W^{39+} become strong at the highest beam energy of 2.00 keV (Fig. 1c) since its ionization potential is 1.8829 keV [18]. While most of the lines are already known from reference [7], it was possible to identify three new lines. In addition, the present accurate measurements allowed us to correct the wavelength of the magnetic-dipole line between the two levels of the ground configuration of $4p^5$. In our previous work [10], where a lower spatial resolution 1320-pixel CCD was used, this transition (Br9) was reported to have a wavelength of (13.474 ± 0.004) nm. As the present measurement was performed with a 2048-pixel CCD and much higher counting statistics, the existence of a strong line at a shorter wavelength of (13.3736 ± 0.0010) nm was very clearly established, as shown in Figure 1c. Moreover, a much more advanced calculation that included more than 2600 atomic levels for W^{39+} results in a theoretical wavelength of 13.383 nm that agrees much better with the experimental value.

The spectral feature labeled Br1 at 4.6813 nm is interpreted here as a blend of 4 transitions. Utter et al. [7] also identified their measured line at 4.68267 nm as a blend although they assigned three transitions to that feature. A fourth line at (4.59539 ± 0.00026) nm in their experiment was associated with a transition with a theoretical wavelength of 4.5669 nm which, from our calculations, is 4.645 nm. We were not able to locate any spectral line close to the measured wavelength from [7], and in addition, the calculated intensities show that the 4.645-nm line is the strongest among all lines of Br-like W.

The line labeled Br7 at 8.1152 nm, which agrees very well with the value of 8.11531 nm from [7], is also a blend of two lines. The stronger component has the same identification as in [7], however, the weaker line seems to contribute some intensity as well, and therefore we added it to the table.

5 Conclusions

Spectroscopy of highly-charged tungsten remains in demand, primarily due to its importance for magnetic fusion research. In the present work we present the measured EBIT spectra in the wavelength range from 2.7 to 17.3 nm and identify transitions in Zr-like W^{34+} to Se-like W^{40+} . These N-shell ions have a large number of electrons and thus are very difficult to model accurately. Nonetheless, our large-scale CR simulations reproduced the experimental spectra fairly well. As a result, we were able to identify 15 new lines in these spectra and corrected identification of a number of spectral lines. Nonetheless, some overlapping lines could not have been unambiguously recognized while some tentatively identified spectral lines show significant disagreement with theory. This situation calls for continuation of spectroscopic measurements of the N-shell ions of tungsten with higher spectral resolution as well as new, higher accuracy calculations.

Acknowledgments

T.D. would like to acknowledge the research grant from the National Institute of Standards and Technology. Y.P. was supported by the NIST NRC Postdoctoral Research Associateships Program.

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Fig. 1.

(a) Observed spectrum of W at 1.65, 1.68, and 1.72 keV electron beam energies. Second and third order spectra are shown in red and green (see text). Asterisks show strong impurity lines from Xe XXVIII at 4.864 nm and Kr XXV at 15.8181 nm [18]. (b) Observed spectrum of W at 1.79, 1.83, and 1.87 keV electron beam energies. Second and third order spectra are shown in red and green (see text). Blue dashed curve represents the spectrometer efficiency curve (in arbitrary units). (c) Observed spectrum of W at 1.90, 1.95, and 2.00 keV electron beam energies. Second and third order spectra are shown in red and green (see text).

Fig. 2.

(a) Comparison of observed and calculated spectra at the electron beam energy of 1.90 keV. The asterisk shows a strong unknown line. (b) Comparison of observed and calculated spectra at the nominal beam energy of 1.95 keV. The asterisk shows an unidentified line.

Table 1.

Experimental and theoretical wavelengths of Zr-like W^{34+} to Se-like W^{40+} . Transition probabilities A (in s^{-1}) are from the present FAC. Notation $A[B]$ for transition probabilities means $A \times 10^B$. The experimental uncertainties in units of the last significant digit of the corresponding wavelength are given in parentheses.

Ion	Key	Lower level	Level No.	Upper level	Level No.	λ_{exp} (nm) Present	λ_{exp} (nm) Reference [7]	λ_{th} (nm) Present	λ_{th} Other	A (s^{-1})	Note ^a	Rel. I_{exp}	Rel. I_{th}
34+	Zr1	$(4d_{-4})_0$	1	$((4d_{-3})_{3/2}, 4f_{-})_1$	202	5.1097(9)		5.088	5.240 ⁺	2.81[12]	N	1.00	1.00
35+	Y1	$(4d_{-3})_{3/2}$	1	$4p_{-}$	217	4.8825(7)		4.461	4.431 [#]	4.20[12]	T	0.93	0.28
	Y2	$(4d_{-3})_{3/2}$	1	$((4d_{-2})_{3/2}, 4f_{-})_{5/2}$	162	5.1255(8)		5.138	5.233 [#]	2.26[12]	N	1.00	1.00
	Y3	$(4d_{-3})_{3/2}$	1	$((4d_{-2})_{3/2}, 4f_{-})_{3/2}$	151	5.4010(9)		5.219	5.311 [#]	2.43[12]	T	0.59	0.83
36+	Sr1	$(4d_{-2})_2$	1	$(4p_{-}, (4d_{-3})_{3/2})_2$	102	4.7683(7)		4.735	4.543 [*]	2.72[12]	N	0.58	0.39
	Sr2	$(4d_{-2})_2$	1	$((4d_{-}, (4f_{-})_{5/2})_3$	86	5.4217(7)		5.365	5.346 [*]	2.49[12]	N	1	1
	Sr3	$(4d_{-2})_0$	2	$((4p_{+}^3)_{3/2}, (4d_{+}^3)_{5/2})_1$	88	5.5652(6) ^b		5.469	5.485 [*]	4.58[11]	T	0.36	0.17
		$(4d_{-2})_0$	2	$(4d_{-}, 4f_{-})_1$	87	5.5652(6) ^b		5.512	5.514 [*]	9.76[11]			0.08
	Sr4	$(4d_{-2})_2$	1	$(4d_{-}, 4f_{-})_2$	66	5.8777(7)		5.846	5.915 [*]	4.46[11]	N	0.19	0.18
	Sr5	$(4d_{-2})_2$	1	$((4p_{+}^3)_{3/2}, (4d_{-}^2)_{7/2}, 4d_{+})_2$	34	6.5711(8)		6.536	6.521 [*]	2.15[11]	T	0.36	0.23
	Sr6	$(4d_{-2})_2$	1	$((4p_{+}^3)_{3/2}, (4d_{-}^2)_{7/2}, 4d_{+})_3$	30	6.7168(7)		6.687	6.752 [*]	1.57[11]	T	0.22	0.35
37+	Rb1	$4d_{-}$	1	$(4p_{-}, (4d_{-}^2)_{3/2})_2$	41	4.5783(8)	4.57810(22)	4.539	4.4766, 4.531 [%]	3.44[12]		0.79	0.99
	Rb2	$4d_{-}$	1	$(4p_{-}, (4d_{-}^2)_{5/2})_2$	34	4.9648(7)	4.96407(54)	4.942	4.9030, 4.922 [%]	1.17[12]		0.83	0.89
	Rb3	$4d_{-}$	1	$4f_{-}$	32	5.6891(8)	5.68797(41)	5.654	5.6055, 5.633 [%]	9.86[11]		0.71	1.46
	Rb4	$4d_{+}$	2	$4f_{+}$	33	6.1901(7) ^b	6.19200(83) ^b	6.145	6.0922, 6.116 [%]	6.05[11]		0.55	0.04
		$4d_{-}$	1	$((4p_{+}^3)_{3/2}, 4d_{-})_{3, (4d_{+})_{1/2}}$	27	6.1901(7) ^b		6.154	6.116 [%]	7.00[11]			0.58
	Rb5	$4d_{+}$	2	$4f_{-}$	32	6.2372(8)	6.19200(83) ^b	6.194	6.1340, 6.167 [%]	1.37[11]		0.35	0.24
	Rb6	$4d_{+}$	2	$((4p_{+}^3)_{3/2}, (4d_{+}^2)_{3/2})_2$	31	6.3428(8) ^b	6.34319(119) ^b	6.285	6.2138, 6.244 [%]	6.47[11]		0.42	0.02
		$4d_{-}$	1	$((4p_{+}^3)_{3/2}, (4d_{+}^2)_{1/2})_2$	26	6.3428(8) ^b		6.288	6.261 [%]	1.45[11]			0.15

Ion	Key	Lower level	Level No.	Upper level	Level No.	λ_{exp} (nm) Present	λ_{exp} (nm) Reference [7]	λ_{th} (nm) Present	λ_{th} Other	A (s^{-1})	Note ^a	Rel. I_{exp}	Rel. I_{th}
Rb		$4d+$	2	$((4p^{+3})_{3/2}, (4d^{+2})_{4/5/2})$	30	6.3428(8) ^b	6.34319(119) ^b	6.294	6.2090, 6.251 [%]	5.90[11]			0.25
	Rb7	$4d-$	1	$((4p^{+3})_{3/2}, 4d^{-})_{3/2}, 4d^{+}$	22	6.4829(10) ^b	6.48250(200)	6.448	6.3775, 6.403 [%]	4.55[11]		1.00	1.00
	Rb8	$4d-$	1	$((4p^{+3})_{3/2}, 4d^{-})_{2/5/2}, 4d^{+}$	20	6.6289(7)	6.629252(147)	6.601	6.5703, 6.570 [%]	1.31[11]		0.71	0.70
	Rb9	$4d+$	2	$((4p^{+3})_{3/2}, 4d^{-})_{2/7/2}, 4d^{+}$	16	7.7075(9)		7.680	7.638 [%]	1.15[07]	N	0.12	0.15
	Rb10	$4d-$	1	$((4p^{+3})_{3/2}, (4d^{-2})_{2/5/2})$	5	8.0142(7) ^b		7.991	7.942 [%]	2.31[09]	N	0.59	0.27
		$4d+$	2	$((4p^{+3})_{3/2}, (4d^{-})_{3/2/1}, (4d^{+})_{5/2/5/2})$	12	8.0142(7) ^b		8.003	7.958 [%]	2.17[09]	N		0.18
	Rb11	$4d+$	2	$((4p^{+3})_{3/2}, (4d^{-})_{3/2/1}, (4d^{+})_{5/2/7/2})$	9	8.1472(8)		8.127	8.080 [%]	3.04[09]	N	0.77	0.22
	Rb12	$4d-$	1	$((4p^{+3})_{3/2}, (4d^{-2})_{2/1/2})$	4	8.1877(10) ^b	8.14573(89) ^b	8.171	8.1299, 8.122 [%]	4.20[09]		0.39	0.12
		$4d-$	1	$((4p^{+3})_{3/2}, (4d^{-2})_{2/3/2})$	3	8.1877(10) ^b	8.14573(89) ^b	8.173	8.1359, 8.123 [%]	1.22[09]			0.20
	Rb13	$4d+$	2	$((4p^{+3})_{3/2}, (4d^{-2})_{0/3/2})$	7	8.6045(8)		8.570	8.514 [%]	1.68[08]	N	0.22	0.20
	Rb14	$4d+$	2	$((4p^{+3})_{3/2}, (4d^{-2})_{2/7/2})$	6	9.0199(8)		8.987	8.918 [%]	7.66[07]	N	0.43	0.72
38+	Kr1	$(4p^{+4})_0$	1	$(4p^{-}, 4d^{-})_1$	12	4.6695(11)	4.66703(12)	4.636	4.6142	2.44[12]		0.81	0.63
	Kr2	$(4p^{+4})_0$	1	$((4p^{+3})_{3/2}, 4d^{+})_1$	9	6.3891(7)	6.38834(41)	6.352	6.3326	6.36[11]		1.00	1.00
	Kr3	$(4p^{+4})_0$	1	$((4p^{+3})_{3/2}, 4d^{-})_1$	3	8.0651(7)	8.06420(226)	8.052	8.0886	2.51[09]		0.71	0.61
39+	Br1	$(4p^{+3})_{3/2}$	1	$((4p^{-}, (4p^{+3})_{3/2/1}, 4d^{+})_{5/2})$	24	4.6813(10) ^b	4.59539(26)	4.645	4.5669	2.69[10]		1.00	1.00
		$(4p^{+3})_{3/2}$	1	$((4p^{-}, (4p^{+3})_{3/2/2}, 4d^{-})_{3/2})$	23	4.6813(10) ^b	4.68267(09) ^b	4.652	4.6181	1.78[12]			0.63
		$(4p^{+3})_{3/2}$	1	$((4p^{-}, (4p^{+3})_{3/2/2}, 4d)_{1/2})$	22	4.6813(10) ^b	4.68267(09) ^b	4.656	4.6069	2.61[12]			0.47
		$(4p^{+3})_{3/2}$	1	$((4p^{-}, (4p^{+3})_{3/2/2}, 4d^{-})_{5/2})$	21	4.6813(10) ^b	4.68267(09) ^b	4.656	4.6188	1.87[12]			0.03
	Br2	$(4p^{+3})_{3/2}$	1	$4s^{+}$	14	6.1047(9)	6.10499(29)	6.083	6.0387	6.43[11]		0.11	0.56
	Br3	$(4p^{+3})_{3/2}$	1	$((4p^{+2})_{2/5/2}, 4d^{+})_{5/2}$	13	6.4672(9)	6.46606(155)	6.437	6.3877	5.68[11]		0.15	1.93

Ion	Key	Lower level	Level No.	Upper level	Level No.	λ_{exp} (nm) Present	λ_{exp} (nm) Reference [7]	λ_{th} (nm) Present	λ_{th} Other	A (s^{-1})	Note ^a	Rel. I_{exp}	Rel. I_{th}
Br4		$(4p^{+3})_{3/2}$	1	$((4p^{+2})_{2,4d}^{+})_{3/2}$	12	6.5681(8)	6.56575(59)	6.538	6.4901	4.09[11]	E	0.15	1.07
Br5		$(4p^{+3})_{3/2}$	1	$((4p^{+2})_{0,4d}^{-})_{3/2}$	7	7.5927(11)		7.581		2.25[08]	N	0.07	0.15
Br6		$(4p^{+3})_{3/2}$	1	$((4p^{+2})_{2,4d}^{-})_{7/2}$	6	7.9011(8)		7.971		1.59[02]	N	0.12	0.37
Br7		$(4p^{+3})_{3/2}$	1	$((4p^{+2})_{2,4d}^{-})_{5/2}$	5	8.1152(9) ^b	8.11531(03)	8.110	8.0892	1.44[09]		0.26	0.95
		$(4p^{+3})_{3/2}$	1	$((4p^{+2})_{2,4d}^{-})_{1/2}$	4	8.1152(9) ^b		8.115		1.09[10]			0.14
Br8		$(4p^{+3})_{3/2}$	1	$((4p^{+2})_{2,4d}^{-})_{3/2}$	3	8.2470(11)		8.235		2.47[09]	N	0.09	0.23
Br9		$(4p^{+3})_{3/2}$	1	$4p^{-}$	2	13.3736(10)		13.383		3.59[06]		0.18	1.54

^aE = blend of Br4 and Se3 in observed spectrum. F = line observed in [7]; now identified as possible blend with Br6. N = new line. T = tentative identification.

The other theoretical wavelengths are from reference [15] unless a superscript is used:

⁺Reference [33].

[#]Reference [32].

^{*}Reference [31].

[%]Reference [30].

Superscript “b” marks blended lines.