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Transition wavelengths and unresolved transition array statistics of ions with $Z = 72 - 89$

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Abstract. Potential extreme ultraviolet and soft X-ray radiation sources have been identified, using the flexible atomic code (FAC), as emission peaks arising from 4d - 4f and 4p - 4d transitions in Pd-like to Rb-like ions of hafnium through actinium. The effects of configuration interaction are investigated and for increasing nuclear charge, these strong emitters are seen to separate and move to shorter wavelength. Each source is characterized using the unresolved transition array model. They are proposed to complement the currently used nitrogen and argon sources in the “water window”, and as possible successors to tin in next generation lithography.

PACS numbers: 31.10.+z, 32.30.Jc, 32.70.-n, 32.80.Aa
1. Introduction

The success of extreme ultraviolet lithography (EUVL) hinges on the ability to identify powerful radiation sources at 13.5 nm, a wavelength at which molybdenum / silicon mirrors are highly reflective [1–4]. To date, both tin and xenon laser produced plasmas (LPPs) and discharge plasmas are the sources of choice at this wavelength: \( \text{Sn}^{8+} - \text{Sn}^{13+} \) emission due to 4d - 4f and 4p - 4d transitions and \( \text{Xe}^{10+} \) emission due to 4d - 5p transitions [1, 4–8]. Many recent research efforts have concentrated on investigating next generation lithographic sources at shorter wavelengths e.g. gadolinium and terbium at 6.75 nm [9–13]. In [14], extreme ultraviolet (EUV) and soft X-ray (SXR) sources were identified at numerous wavelengths with the prospect of being used in the event of a highly reflective mirror becoming available at any of these wavelengths.

Moving to shorter wavelengths, further into the SXR region, we enter what is known as the “water window” (2.3–4.4 nm), where live biological sampling is desirable [15, 16]. Current sources in this region are strong quasi-monochromatic emission at \( \lambda = 2.879 \) nm and \( \lambda = 2.478 \) nm wavelengths arising from 1s\(^2\) - 1s 2p in \( \text{N}^{5+} \) and 1s - 2p in \( \text{N}^{6+} \) respectively, and broadband emission between \( \lambda = 2 - 4 \) nm from argon gas targets [15]. Quasi-monochromatic sources are suitable for biological imaging using diffractive optics while broadband emission sources can be used for contact microscopy. The development of compact, high repetition rate, table top SXR sources using these gas puff targets, which have the advantage of being debris free, provide much needed laboratory \textit{in situ} alternatives to free electron lasers and synchrotrons and can be used in numerous experiments, e.g. microscopy, spectroscopy and metrology.

It is proposed that the sources identified in this work would be generated in laser produced plasmas (LPPs), where a solid target is irradiated with an intense laser pulse. This however leads to the production of debris which can cause major degradation of expensive EUV / SXR mirrors. Different techniques to minimize debris have been proposed [2] such as mixed composition targets [17, 18] and liquid tin mirrors as collectors [19]. Indeed it may be possible to extend these approaches into the SXR region, e.g. the liquid tin mirror being developed for 13.5 nm could be a prototype for elements at other wavelengths.

The recording of the 4d - 4f emission in cesium through lutetium showed that these relatively narrow regions of resonance-like emission became more complex and moved to shorter wavelength with increasing nuclear charge \( Z \) [20, 21]. In order to interpret such complicated spectra, Mandelbaum \textit{et al} [22] employed the unresolved transition array (UTA) approach developed by Bauche-Arnoult, Bauche and Klapisch [23–26] and concluded that interactions between the \( 4p^6 \) 4d\(^{N-1}\) 4f and \( 4p^5 \) 4d\(^{N+1}\) configurations are responsible for narrowing the transition arrays and their superposition in adjacent ion stages. In this work we adopt the UTA approach to characterize the emission arising from 4d - 4f and 4p - 4d transitions in Pd-like to Rb-like ions of hafnium through actinium (\( Z = 72 – 89 \)). Of these elements tungsten and gold have received most attention to date owing to their use in the fusion community [27–31]. Tungsten is currently being
used in the walls of the divertor in many magnetic confinement fusion devices, such as tokamaks, to reduce tile erosion [29, 32, 33]. However even small quantities of tungsten contaminating the core plasma (> $10^{-5}$ [34]) can seriously limit the energy confinement in a fusion reactor. Knowledge of the W emission radiated from each ion stage in the plasma core is therefore essential to eradicate this degradation. Gold is used for indirectly driven inertial confinement fusion (ICF), where laser radiation heats the inside of a Au hohlraum producing a plasma which emits intense x-rays. Therefore knowledge of Au radiative opacity is crucial to the success of ICF [30, 31].

Recent experiments have employed the LPP technique using metal targets to generate EUV/SXR radiation. For example a bulk rhenium target was used to develop new SXR microscopy applications in the "carbon window" ($\lambda \approx 4.5 - 5$ nm) [35]. Also a solid gold-based LPP source was utilized in the design of an EUV source and optics setup to achieve high energy density and spatial resolution in a compact setup [36]. In [37] the emitted X-ray spectra of different target materials were recorded over the wavelength range of 0.8–18 nm. Low-Z elements (Cu, Ti, Fe, and Al) resulted in intense line emission, while continuum-like emission was detected from higher-Z materials (Mo and Ag). Therefore it is possible to optimize the brilliance of the LPP source for a specific x-ray emission range and a particular application of interest.

The outline of this paper is as follows: In section 2, 180 theoretical 4d - 4f and 4p - 4d unresolved transition array (UTA) spectra are presented, for ions with configurations $4p^6 4d^N - 4p^6 4d^{N+1}$ and $4p^5 4d^N - 4p^5 4d^{N+1}$, $N = 1..10$. The effects of configuration interaction (CI), and overall trends in the position and intensity of UTA peaks from hafnium to actinium are discussed. In section 3 UTA statistics, namely, mean wavelength $\bar{\lambda}_{gA}$ and spectral width $\Delta \lambda_{gA}$ for the above ions are calculated which allows us to characterize these possible EUV / SXR sources. The gradual separation of the 4d - 4f UTA from the 4p - 4d UTA is highlighted. Finally in section 4 we conclude with a summary of this work.

2. Unresolved Transition Arrays of Ions with $Z = 72 - 89$

As noted in [14] the strongest lines occurring in the EUV result from 4d - 4f and 4p - 4d transitions in ion stages with open 4d subshells. Calculations were performed with the flexible atomic code (FAC) [38, 39], a complete software package developed for the computation of various atomic collisional and radiative processes to model spectral emission from astrophysical plasmas. Since its introduction however it has been successfully applied in numerous additional fields e.g. magnetic fusion and laser produced plasmas. FAC combines the strengths of existing atomic codes e.g. ATOM [40], HULLAC [41] and SZ [42, 43]; it uses a fully relativistic approach based on the Dirac equation, and implements efficient methods for distorted wave approximation, thus allowing its application to ions with large values of nuclear charge. The following basis set was used: $4p^6 4d^N$, $4p^6 4d^{N-1} nl$ and $4p^5 4d^{N+1}$ where $n \leq 8$, $l \leq 3$ and $1 \leq N \leq 10$. Figures 1 - 3 show Pd-like through Rb-like spectra of hafnium through
actinium including CI. 4d - 4f transitions are shown in black, 4p - 4d transitions are shown in orange (gray) and all other transitions are shown in yellow (light gray). It was noted in [14] that for a given element, the emission from 4d - 4f and 4p - 4d becomes stronger and more concentrated within a particular wavelength range when configuration interaction is included. It is well known that CI redistributes transitions providing a more accurate description of experimental spectra [44]. However as $Z$ increases there was little discernable difference between the spectra excluding CI and including CI. This point will be further developed under the UTA framework in section 3. Figure 4 displays the maximum peak emission (in terms of gA values) for (a) 4d - 4f transitions and (b) 4p - 4d transitions for each element as a function of wavelength. As was observed for the lanthanides [14, 20–22], both 4d - 4f and 4p - 4d emission moves to shorter wavelength on increasing $Z$. The dependence of peak transition energies on atomic number $Z$ is presented in Figure 4 (c). This shows that on increasing $Z$, the 4d - 4f emission peak and the 4p - 4d emission peak clearly separate. However, the fact that the maximum gA value remains relatively comparable for each transition type over the range of $Z = 72 – 89$, implies that these elements could be potential radiation sources over the wavelength range $\lambda = 2.5 – 6$ nm. This point is further quantified with the aid of UTA statistical analysis in the following section.

3. Unresolved Transition Array Statistics of Ions with $Z = 72 – 89$

In order to quantify the emission from the 4d - 4f and 4p - 4d transitions in these ions, we adopted the unresolved transition array (UTA) approach developed by Bauche-Arnoult, Bauche and Klapisch [23–26]. UTAs were introduced originally to aid interpretation of low resolution soft X-ray spectra emitted by hot plasmas. They are currently widely used to approximate complex atomic spectra in plasma opacity and emissivity calculations which reduces computation times in large-scale radiation hydrodynamic simulations of plasma dynamics. In the UTA model, the discrete line spectra are replaced by a continuous function (usually Gaussian) such that each configuration-configuration transition array is characterized by the average quantities such as total intensity, average transition energy and variance. The average and variance of the transition energies ($\bar{E}$ and $\sigma^2$ respectively) can be expressed as the gA-weighted sums

$$\bar{E} = \frac{\sum_{j<i} g_j A_{ji} E_{ij}}{\sum_{j<i} g_j A_{ji}}$$

(1)

and

$$\sigma^2 = \frac{\sum_{j<i} g_j A_{ji} (\bar{E} - E_{ij})^2}{\sum_{j<i} g_j A_{ji}}$$

(2)

where $A_{ji}$ is the Einstein coefficient for spontaneous emission from level $j$ to level $i$, and $g_j$ is the statistical weight of the upper level. The mean wavelength $\bar{\lambda}_{gA}$ and the
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The spectral width $\Delta \lambda_{gA}$ of the transition array can be defined as follows

$$\bar{\lambda}_{gA} = \frac{10^8}{\bar{E}},$$  

$$\Delta \lambda_{gA} = \sqrt{8\ln 2} \times 10^8 \sigma / \bar{E}^2,$$

where $\bar{E}$ and $\sigma$ are expressed in $cm^{-1}$ and $\bar{\lambda}_{gA}$ and $\Delta \lambda_{gA}$ in $\AA$.

Before applying the above UTA analysis, it is worthwhile to demonstrate the accuracy of the FAC code and the validity of its use in the current work. As an example, the $4p^6\ 4d - 4p^5\ 4d^2$ and $4p^6\ 4d - 4p^6\ 4f$ transition wavelengths and UTA statistics of the Rb-like tungsten ion, $W^{37+}$ are presented in Table 1. This is a suitable choice owing to recent interest in it by members of the fusion community. As such wavelengths from a number of sources are available and it can be seen that the results of the current theoretical work compare favorably with experimentally recorded values. The $4p^6\ 4d - 4p^5\ 4d^2$ and $4p^6\ 4d - 4p^6\ 4f$ transitions were first identified by Radtke et al [29] using an electron-beam ion trap at a wavelength uncertainty of $\pm 0.05\AA$. Later Utter et al [45] improved on this by recording at a higher spectral resolution with wavelength uncertainties of between $\pm 0.004$ and $\pm 0.02\AA$. In the work of Radtke et al [29], $ab\ initio$ theoretical calculations were carried out using the multiconfigurational relativistic HULLAC code [46, 47] and the difference between measured and calculated wavelengths was found to be as much as 1\AA. The current calculations employ the FAC code which has an accuracy of 10 - 30 m\AA at 10\AA [48]. The wavelengths calculated with the FAC code are in closer agreement with experimental values, where the largest difference is found to be 0.6\AA. Also presented in Table 1 is the UTA analysis for $W^{37+}$ where (i) denotes the results of Radtke et al [29] obtained using the HULLAC code, and (ii) refers to results obtained by application of 1- 4 to the FAC data produced in the current work. Agreement is good with a maximum difference of 0.16\AA in the spectral width of the mixed CI transition array ($4p^6\ 4d - [4p^5\ 4d^2 + 4p^6\ 4f]$). This can be attributed to the use of a larger basis set in the current work, as described in Section 2. As was the approach in [12], this basis set was chosen for consistency when surveying such a large number of ions. Inclusion of various configurations will continue as and when more detailed experimental energy levels, transition wavelengths and line strengths of these ions become available for comparison.

The above discussion indicates that the use of the FAC code is appropriate for producing the 180 theoretical ionic spectra considered here. It also shows that these spectra can be adequately described using the UTA approach. The 4d - 4f and 4p - 4d UTAs were extracted from the CI spectra and the above statistical analysis was applied to each separately. The results are displayed in Figure 5, excluding CI (left) and including CI (right), and Tables 2 and 3. Figure 5 shows the dependence of mean wavelength ($\bar{\lambda}_{gA}$) on ion stage for each element with $Z = 72 – 89$ (4d - 4f in black and 4p - 4d in red). A number of observations can be made from these results: (i) CI effects are more dramatic in lower $Z$ elements, (ii) CI concentrates the 4p - 4d UTA at a particular wavelength for this series of ions, for example, in hafnium which is plotted...
in Figure 5 (c) non-CI and (d) CI. For the 4p - 4d UTA, $\bar{\lambda}_{gA}$ varies from 5.29 - 5.86 nm in the non-CI case compared to 5.17 - 4.82 nm in the CI case. For the 4d - 4f UTA, $\bar{\lambda}_{gA}$ varies from 6.43 - 5.09 nm in the non-CI case compared to 6.26 - 5.06 nm in the CI case. (iii) CI effects the 4p - 4d UTA positioning more than the 4d - 4f in hafnium. This can be observed for many of the lower $Z$ elements in this study. Gradually the effects of CI are diminished as can be seen by comparing Figure 5 (a) and (b). Finally by actinium we see very little variation between CI and non-CI results. For the 4p - 4d UTA, $\bar{\lambda}_{gA}$ varies from 2.79 - 2.98 nm in the non-CI case compared to 2.77 - 2.54 nm in the CI case. For the 4d - 4f UTA, $\bar{\lambda}_{gA}$ varies from 4.27 - 3.40 nm in the non-CI case compared to 3.88 - 3.39 nm in the CI case. These results are summarized for the CI case only in Tables 2 and 3. The mean wavelength $\bar{\lambda}_{gA}$ and spectral width $\Delta \lambda_{gA}$ for 4d - 4f and 4p - 4d UTAs calculated from the CI spectra are presented. From these values and the results presented in Figure 4, it is possible to identify strong emitters for almost all wavelengths between approximately $\lambda = 2.5 - 6$ nm. Indeed in some cases it is possible that a target of mixed composition may give broad band emission across this wavelength range encompassing the “water window” and soft X-ray region.

4. Conclusion

Possible extreme ultraviolet and soft X-ray radiation sources were identified, using the FAC relativistic code, as emission peaks arising from 4d - 4f and 4p - 4d transitions in Pd-like to Rb-like ions of hafnium through actinium. For increasing nuclear charge, these strong emitters are seen to separate and move to shorter wavelength. The emission was comparable from each source and was characterized using the unresolved transition array model. The laser produced plasma technique may be employed in future work to generate these radiation sources which find application in numerous exciting fields, e.g. microscopy, spectroscopy and lithography.

Acknowledgments

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**Figure 1.** (Color online) Pd-like through Rb-like spectra of hafnium through iridium computed with the FAC code including CI. Black denotes 4d - 4f transitions, orange (gray) denotes 4p - 4d transitions and yellow (light gray) denotes all transitions.
Figure 2. (Color online) Pd-like through Rb-like spectra of platinum through bismuth computed with the FAC code including CI. Black denotes 4d - 4f transitions, orange (gray) denotes 4p - 4d transitions and yellow (light gray) denotes all transitions.
Figure 3. (Color online) Pd-like through Rb-like spectra of polonium through actinium computed with the FAC code including CI. Black denotes 4d - 4f transitions, orange (gray) denotes 4p - 4d transitions and yellow (light gray) denotes all transitions.
Figure 4. (Color online) Maximum peak emission from (a) 4d - 4f and (b) 4p - 4d UTAs (including CI) in elements with $Z = 72 - 89$. (c) Dependence of UTA transition energies on atomic number $Z$, 4d - 4f (black open circles), 4p - 4d (red crosses).
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Figure 5. (Color online) Dependence of mean wavelength ($\bar{\lambda}_{gA}$) on ion stage for elements with $Z = 72 - 89$ (4d - 4f UTA black dot, 4p - 4d UTA red cross): (a) tantalum through radium non-CI, (b) tantalum through radium CI, (c) hafnium non-CI, (d) hafnium CI, (e) actinium non-CI and (f) actinium CI.
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Table 1. Transition wavelengths and UTA statistics of Rb-like tungsten, W$^{37+}$.

(a) Transition wavelengths: In column (i) $\lambda_{exp}$ and $\lambda_{th}$ respectively, denote the experimental and theoretical transition wavelengths obtained by Radtke et al. [29]. The theoretical values were calculated using the HULLAC code. In column (ii) $\lambda_{th}$ denotes theoretical wavelengths calculated in the present work using the FAC code. In column (iii) $\lambda_{exp}$ refers to transition wavelengths recorded experimentally by Utter et al. [45] and presented by Kramida and Shirai in [49].

(b) UTA statistics: Calculated mean wavelength $\bar{\lambda}_{gA}$ and spectral width $\Delta \lambda_{gA}$ for the unresolved transition arrays. Column (i) denotes values from Radtke et al. [29] and column (ii) denotes values obtained by applying 1-4 to the FAC data produced in the current work. Wavelengths throughout the table are given in Å.

| Transition | (i) $\lambda_{exp}$ | (ii) $\lambda_{th}$ | (iii) $\lambda_{exp}$ |
|------------|---------------------|---------------------|---------------------|
| 4p$^6$ 4d $^2D_{3/2} - 4p^5(2P_{1/2})$ 4d$^2$($^3F_2$) (1/2, 2, 2)$_{5/2}$ | 49.52 | 49.06 | 49.32 | 49.641 |
| 4p$^6$ 4d $^2D_{3/2} - 4p^6$ 4f (0, 5/2) $_5/2$ | 56.86 | 56.04 | 56.46 | 56.880 |
| 4p$^6$ 4d $^2D_{3/2} - 4p^5(2P_{3/2})$ 4d$^2$($^3F_4$) (3/2, 4)$_{5/2}$ | 57.74 | 56.72 | 57.16 | 57.755 |
| 4p$^6$ 4d $^2D_{3/2} - 4p^5(2P_{3/2})$ 4d$^2$($^3F_3$) (3/2, 3)$_{3/2}$ | 64.82 | 63.87 | 64.40 | 64.825 |

| Unresolved transition array | (i) $\lambda_{gA}$ | (ii) $\Delta \lambda_{gA}$ | (iii) $\lambda_{gA}$ | $\Delta \lambda_{gA}$ |
|----------------------------|-------------------|---------------------|---------------------|
| 4p$^6$ 4d - 4p$^5$ 4d$^2$ | 49.18 | 14.28 | 49.23 | 14.22 |
| 4p$^6$ 4d - 4p$^6$ 4f | 60.93 | 5.15 | 60.96 | 5.18 |
| Mixed | 49.00 | 13.16 | 49.01 | 13.00 |
Table 2. Calculated mean wavelength $\bar{\lambda}_{gA}$ and spectral width $\Delta\lambda_{gA}$ for the configuration interaction unresolved transition arrays of hafnium through mercury ions: Rb-like to Rh-like ions for the 4p - 4d arrays and Rb-like to Pd-like ions for the 4d - 4f arrays. Wavelengths throughout the table are given in Å.

| Ion   | $\lambda_{gA}$ | $\Delta\lambda_{gA}$ | $\bar{\lambda}_{gA}$ | $\Delta\lambda_{gA}$ |
|-------|----------------|-----------------------|------------------------|------------------------|
| 4p - 4d | Hf  | Ta  | W  | Re  | Os  | Ir  | Pt  | Au  | Hg  |
| Rb-like | 51.72 | 11.13 | 49.87 | 11.21 | 48.03 | 11.06 | 46.29 | 11.02 | 43.86 | 9.21 | 42.85 | 10.94 | 41.29 | 11.02 | 39.78 | 11.03 | 38.31 | 10.98 |
| Sr-like | 50.52 | 6.94 | 48.57 | 6.73 | 47.10 | 8.08 | 45.44 | 8.48 | 43.62 | 8.08 | 41.92 | 7.91 | 40.63 | 8.83 | 39.07 | 8.62 | 37.49 | 8.40 |
| Y-like | 50.31 | 6.22 | 48.27 | 5.68 | 46.49 | 5.89 | 44.83 | 6.33 | 43.13 | 6.33 | 41.63 | 6.80 | 39.95 | 6.33 | 38.57 | 6.84 | 37.11 | 6.72 |
| Zr-like | 50.26 | 6.01 | 48.02 | 4.79 | 46.22 | 4.85 | 44.41 | 4.42 | 42.70 | 4.35 | 41.06 | 4.21 | 39.46 | 3.79 | 37.98 | 3.43 | 36.88 | 5.65 |
| Nb-like | 50.06 | 5.87 | 48.20 | 5.76 | 46.07 | 4.73 | 44.19 | 4.06 | 42.56 | 4.21 | 40.92 | 3.93 | 39.32 | 3.43 | 37.87 | 3.65 | 36.38 | 3.13 |
| Mo-like | 49.59 | 5.58 | 47.86 | 5.62 | 46.16 | 5.58 | 44.31 | 5.03 | 42.27 | 3.45 | 40.68 | 3.22 | 39.16 | 3.19 | 37.65 | 2.67 | 36.25 | 2.84 |
| Tc-like | 49.28 | 5.70 | 47.37 | 5.28 | 45.66 | 5.23 | 44.20 | 5.43 | 42.41 | 4.97 | 40.65 | 4.15 | 38.94 | 2.78 | 37.49 | 2.70 | 36.09 | 2.53 |
| Ru-like | 48.47 | 5.17 | 46.81 | 5.24 | 45.06 | 4.85 | 43.19 | 3.02 | 41.70 | 3.52 | 40.19 | 3.34 | 38.70 | 2.66 | 37.29 | 2.51 | 35.92 | 2.35 |
| Rh-like | 48.24 | 7.28 | 46.65 | 7.36 | 44.56 | 5.26 | 43.01 | 5.11 | 41.51 | 4.95 | 40.04 | 4.77 | 38.62 | 4.57 | 37.23 | 4.35 | 35.88 | 4.09 |

| 4d - 4f | Hf  | Ta  | W  | Re  | Os  | Ir  | Pt  | Au  | Hg  |
|----------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| Rb-like | 62.60 | 5.70 | 60.85 | 5.84 | 59.35 | 5.95 | 58.17 | 5.90 | 56.35 | 6.05 | 54.44 | 5.77 | 52.77 | 5.65 | 51.29 | 5.56 | 49.93 | 5.49 |
| Sr-like | 60.90 | 8.55 | 59.28 | 8.24 | 57.42 | 8.00 | 55.69 | 7.51 | 54.32 | 7.35 | 52.93 | 7.09 | 51.40 | 6.85 | 50.26 | 6.64 | 48.82 | 6.29 |
| Y-like | 58.31 | 7.92 | 56.77 | 7.54 | 55.30 | 7.18 | 53.83 | 6.59 | 52.38 | 6.35 | 51.11 | 6.40 | 49.92 | 6.32 | 48.65 | 6.12 | 47.53 | 5.98 |
| Zr-like | 56.06 | 6.22 | 54.74 | 5.99 | 53.39 | 5.72 | 52.10 | 5.67 | 50.79 | 5.45 | 49.61 | 5.39 | 48.44 | 5.36 | 47.31 | 5.34 | 46.14 | 5.16 |
| Nb-like | 54.34 | 4.01 | 53.11 | 4.15 | 51.89 | 4.25 | 50.65 | 4.22 | 49.39 | 4.08 | 48.23 | 4.11 | 47.13 | 4.26 | 46.02 | 4.20 | 45.00 | 4.34 |
| Mo-like | 53.42 | 2.66 | 52.06 | 2.80 | 50.76 | 2.85 | 49.57 | 3.15 | 48.40 | 3.24 | 47.23 | 3.25 | 46.13 | 3.38 | 45.07 | 3.47 | 44.03 | 3.49 |
| Tc-like | 52.64 | 1.80 | 51.26 | 1.92 | 49.95 | 2.06 | 48.70 | 2.16 | 47.49 | 2.21 | 46.38 | 2.49 | 45.29 | 2.60 | 44.24 | 2.75 | 43.24 | 2.97 |
| Ru-like | 51.94 | 1.51 | 50.56 | 1.51 | 49.24 | 1.54 | 48.01 | 1.86 | 46.83 | 2.05 | 45.69 | 2.12 | 44.60 | 2.32 | 43.56 | 2.50 | 42.53 | 2.44 |
| Rh-like | 51.23 | 0.58 | 49.85 | 0.56 | 48.57 | 1.33 | 47.33 | 1.34 | 46.13 | 1.34 | 45.02 | 1.77 | 43.95 | 2.03 | 42.90 | 2.05 | 41.95 | 2.62 |
| Pd-like | 50.56 | 0.00 | 49.19 | 0.00 | 47.89 | 0.00 | 46.74 | 2.13 | 45.56 | 2.18 | 44.44 | 2.23 | 43.36 | 2.28 | 42.33 | 2.33 | 41.34 | 2.38 |
Table 3. Calculated mean wavelength $\bar{\lambda}_{gA}$ and spectral width $\Delta \lambda_{gA}$ for the configuration interaction unresolved transition arrays of thallium through actinium ions: Rb-like to Rh-like ions for the 4p - 4d arrays and Rb-like to Pd-like ions for the 4d - 4f arrays. Wavelengths throughout the table are given in Å.

| Ion    | 4p - 4d | Tl | Pb | Bi | Po | At | Rn | Fr | Ra | Ac |
|--------|---------|----|----|----|----|----|----|----|----|----|
|        | $\bar{\lambda}_{gA}$ | $\Delta \lambda_{gA}$ | $\bar{\lambda}_{gA}$ | $\Delta \lambda_{gA}$ | $\bar{\lambda}_{gA}$ | $\Delta \lambda_{gA}$ | $\bar{\lambda}_{gA}$ | $\Delta \lambda_{gA}$ | $\bar{\lambda}_{gA}$ | $\Delta \lambda_{gA}$ |
| Rb-like | 36.90   | 10.93 | 35.54 | 10.85 | 34.20 | 10.71 | 32.92 | 10.58 | 32.30 | 12.09 | 31.08 | 11.91 | 29.91 | 11.72 | 28.76 | 11.50 | 27.66 | 11.28 |
| Sr-like | 36.36   | 9.21  | 35.09 | 9.40  | 33.68 | 9.06  | 32.61 | 9.58  | 31.42 | 9.52  | 30.19 | 9.29  | 29.16 | 9.49  | 28.26 | 9.93  | 27.18 | 9.74  |
| Y-like  | 35.59   | 6.08  | 34.35 | 6.51  | 33.19 | 7.16  | 31.90 | 6.93  | 30.67 | 6.85  | 29.54 | 6.98  | 28.63 | 7.69  | 27.80 | 8.42  | 26.65 | 8.09  |
| Zr-like | 35.35   | 5.12  | 34.14 | 5.61  | 32.77 | 5.21  | 31.58 | 5.49  | 30.44 | 5.70  | 29.43 | 6.28  | 28.36 | 6.42  | 27.58 | 7.34  | 26.35 | 6.77  |
| Nb-like | 35.08   | 3.62  | 33.78 | 3.73  | 32.44 | 3.22  | 31.29 | 3.83  | 30.24 | 4.69  | 29.06 | 4.55  | 28.06 | 5.04  | 26.90 | 4.58  | 36.06 | 5.50  |
| Mo-like | 34.90   | 2.83  | 33.57 | 2.71  | 32.36 | 3.15  | 31.11 | 2.78  | 29.98 | 3.15  | 29.12 | 4.65  | 27.72 | 4.15  | 26.81 | 3.91  | 25.83 | 4.30  |
| Tc-like | 34.74   | 2.34  | 33.42 | 2.01  | 32.15 | 1.71  | 30.97 | 1.92  | 29.77 | 1.59  | 28.65 | 1.54  | 27.54 | 1.31  | 26.67 | 3.17  | 25.74 | 3.61  |
| Ru-like | 34.59   | 2.17  | 33.28 | 1.33  | 32.04 | 1.25  | 30.85 | 1.18  | 29.69 | 1.11  | 28.58 | 1.04  | 27.50 | 0.98  | 26.45 | 0.92  | 25.44 | 0.86  |
| Rh-like | 34.57   | 3.78  | 33.29 | 3.42  | 31.91 | 0.00  | 30.74 | 0.00  | 29.75 | 3.11  | 28.65 | 3.11  | 27.58 | 3.02  | 26.53 | 2.84  | 25.41 | 0.00  |

| Ion    | 4d - 4f | Tl | Pb | Bi | Po | At | Rn | Fr | Ra | Ac |
|--------|---------|----|----|----|----|----|----|----|----|----|
|        | $\bar{\lambda}_{gA}$ | $\Delta \lambda_{gA}$ | $\bar{\lambda}_{gA}$ | $\Delta \lambda_{gA}$ | $\bar{\lambda}_{gA}$ | $\Delta \lambda_{gA}$ | $\bar{\lambda}_{gA}$ | $\Delta \lambda_{gA}$ | $\bar{\lambda}_{gA}$ | $\Delta \lambda_{gA}$ |
| Rb-like | 48.65   | 5.43  | 47.43 | 5.38  | 46.24 | 5.29  | 45.13 | 5.24  | 42.29 | 0.00  | 41.26 | 0.00  | 40.27 | 0.00  | 39.31 | 0.00  | 38.38 | 0.00  |
| Sr-like | 47.39   | 5.99  | 46.24 | 5.84  | 45.16 | 5.79  | 43.92 | 5.60  | 42.97 | 5.66  | 41.97 | 5.49  | 40.87 | 5.30  | 39.85 | 4.76  | 38.83 | 4.74  |
| Y-like  | 46.51   | 6.01  | 45.41 | 5.84  | 44.20 | 5.63  | 43.24 | 5.54  | 42.17 | 5.40  | 41.15 | 5.27  | 40.09 | 5.02  | 39.09 | 4.80  | 38.12 | 4.60  |
| Zr-like | 45.03   | 5.02  | 44.01 | 4.94  | 43.06 | 5.04  | 42.07 | 5.05  | 41.10 | 4.94  | 40.18 | 4.86  | 39.29 | 4.82  | 38.44 | 4.78  | 37.55 | 4.72  |
| Nb-like | 43.97   | 4.31  | 42.99 | 4.39  | 42.04 | 4.44  | 41.10 | 4.41  | 40.16 | 4.31  | 39.28 | 4.33  | 38.43 | 4.34  | 37.60 | 4.35  | 36.74 | 4.22  |
| Mo-like | 43.03   | 3.56  | 42.05 | 3.56  | 41.10 | 3.56  | 40.22 | 3.69  | 39.34 | 3.73  | 38.48 | 3.75  | 37.65 | 3.80  | 36.86 | 3.87  | 36.06 | 3.85  |
| Tc-like | 42.23   | 2.92  | 41.29 | 3.05  | 40.37 | 3.08  | 39.48 | 3.10  | 38.63 | 3.21  | 37.84 | 3.50  | 37.01 | 3.46  | 36.23 | 3.54  | 35.46 | 3.54  |
| Ru-like | 41.57   | 2.62  | 40.64 | 2.74  | 39.74 | 2.87  | 38.87 | 2.95  | 38.02 | 3.00  | 37.20 | 3.06  | 36.42 | 3.16  | 35.66 | 3.28  | 34.92 | 3.35  |
| Rh-like | 40.95   | 2.34  | 40.04 | 2.57  | 39.19 | 2.91  | 38.33 | 2.98  | 37.50 | 3.04  | 36.69 | 3.09  | 35.91 | 3.14  | 35.15 | 3.19  | 34.42 | 3.22  |
| Pd-like | 40.39   | 2.43  | 39.47 | 2.48  | 38.59 | 2.54  | 37.74 | 2.59  | 36.92 | 2.64  | 36.12 | 2.69  | 35.35 | 2.74  | 34.61 | 2.78  | 33.89 | 2.83  |