Partial and total dielectronic recombination rate coefficients for \(W^{55+}\) to \(W^{38+}\)

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Abstract

Dielectronic recombination (DR) is the dominant mode of recombination in magnetically confined fusion plasmas for intermediate to low-charged ions of W. Complete, final-state resolved partial isonuclear W DR rate coefficient data is required for detailed collisional-radiative modelling for such plasmas in preparation for the upcoming fusion experiment ITER. To realise this requirement, we continue The Tungsten Project by presenting our calculations for tungsten ions \(W^{55+}\) to \(W^{38+}\). As per our prior calculations for \(W^{73+}\) to \(W^{56+}\), we use the collision package AUTOSTRUCTURE to calculate partial and total DR rate coefficients for all relevant core-excitations in intermediate coupling (IC) and configuration average (CA) using \(\kappa\)-averaged relativistic wavefunctions. Radiative recombination rate coefficients are also calculated for the purpose of evaluating ionisation fractions. Comparison of our DR rate coefficients for \(W^{46+}\) with other authors yields agreement to within 7%–19% at peak abundance verifying the reliability of our method. Comparison of partial DR rate coefficients calculated in IC and CA yield differences of a factor \(~2\) at peak abundance temperature, highlighting the importance of relativistic configuration mixing. Large differences are observed between ionisation fractions calculated using our recombination rate coefficient data and that of Pütterich et al (2008 Plasma Phys. Control. Fusion 50 085016). These differences are attributed to deficiencies in the average-atom method used by the former to calculate their data.

Keywords: dielectronic recombination, electron–ion collisions, finite-density plasmas

(Some figures may appear in colour only in the online journal)

1. Introduction

The upcoming experimental fusion reactor ITER1 is currently being constructed in Cadarache, France. Scheduled for a first plasma in December 20252, ITER has been designed with the aim of producing ten times as much energy as it consumes for operations. The reactor wall of ITER will be constructed with beryllium tiles, and the divertor will be composed of tungsten [1]. In preparation for the experiments that will take place at ITER, the Joint European Torus (JET) based in Culham, Oxford, has been fitted with an ITER-like wall [2]. In addition, the ASDEX upgrade [3] now uses nearly 100% tungsten in its set-up. Tungsten has been chosen for its ability to withstand large power loads even in the presence of micro-fractures, resistance to tritium absorption [4], and high melting point. However, being a plasma facing component, tungsten will sputter from the divertor into the main body plasma, potentially cooling and quenching the plasma. The power loss [5] arising from the presence of tungsten impurities can be calculated using sophisticated collisional-radiative (CR) models [6]. Partial final-state resolved DR rate coefficients are required not just for high-\(n\) but also for population modelling of low-lying energy levels. As input, CR models require accurate isonuclear partial final-state resolved dielectronic recombination (DR) rate coefficient data for the elements being included.

Several calculations have been performed in response to the demand for tungsten DR rate coefficient data. The first attempt at a baseline set of data was done by [7, 8] using an

\(^1\) http://iter.org
\(^2\) https://iter.org/newsline/-/2482
average-atom method, ADPAK. 27 years later, tungsten DR rate coefficient data3 was calculated using the relativistic configuration average (CA) code FLYCHK [9]. Next, Foster [10] used the Burgess General Formula [11] to calculate data for tungsten. Finally, Pütterich et al [12] used the data of ADPAK, but multiplied the DR rate coefficients of several ionisation stages (W\textsuperscript{22+} – W\textsuperscript{55+}) by empirical scaling factors to alter the theoretical ionisation balance and improve agreement with observed spectral emission. Both Foster and Pütterich et al used scaled hydrogenic recombination (RR) rate coefficients. While these approaches cover the iononuclear sequence, agreement between the three methods is lacking. For example, in figure 1 we show the recombination rate coefficients for W\textsuperscript{44+} as calculated by Pütterich et al, Foster, and Chung et al. It can be seen there is little-to-no similarity between the results of the three calculations. At the very least, the variation between the three curves give an indication on the uncertainty on the data, however, this is not very useful for calculating detailed CR models.

Large uncertainties in calculated recombination rate coefficients translate to uncertainties in peak abundance temperatures. In figure 1 of [13] we plotted the tungsten ionisation balance calculated using the ionisation rate coefficients of Loch et al [14], and the recombination rate coefficients of Foster and Pütterich et al. It was shown that while there is moderate agreement for the ten highest ionisation stages where RR is dominant, the position of and size of the fractions for each ionisation stage differs markedly.

Calculating final-state resolved partial DR rate coefficients is a more involved process, and has only been done for a select few ionisation stages of tungsten. Typically, the ionisation stages considered have been for simpler cases where the electron shell is near- or completely filled, however, there are exceptions. To date, the most complex tungsten ions to have been studied are the open-f shell ions W\textsuperscript{18+}, W\textsuperscript{19+}, and W\textsuperscript{20+} (4f\textsuperscript{0}{4f\textsuperscript{q}, q = 8, 9, 10}) by Spruck et al and Badnell et al [15–17] using an updated version of AUTOSTRUCTURE to cope with the large number of levels. A less computationally demanding set of calculations were carried out by Preval et al [13], who also used AUTOSTRUCTURE to calculate partial and total DR rate coefficients for W\textsuperscript{73+} to W\textsuperscript{56+} as part of The Tungsten Project. The RR rate coefficients were also calculated alongside these for use in ionisation balance comparisons.

In addition to our calculations using AUTOSTRUCTURE, other codes have been used to calculate detailed DR rate coefficients for tungsten. Behar et al used the HULLAC code [18] and the Cowan code [19] to calculate DR rate coefficients for W\textsuperscript{46+}, W\textsuperscript{45+}, W\textsuperscript{56+} [20, 21], and W\textsuperscript{64+} [22]. Peleg et al [23] also used HULLAC and the Cowan Code to calculate DR rate coefficients for W\textsuperscript{56+}. In addition, Safonova et al has used HULLAC to calculate DR rate coefficients for W\textsuperscript{44+}, W\textsuperscript{66+}, W\textsuperscript{34+}, W\textsuperscript{45+}, W\textsuperscript{46+}, W\textsuperscript{43+}, and W\textsuperscript{54+} [24–30]. The flexible atomic code (FAC) [31] was used by Li et al to calculate DR rate coefficients for W\textsuperscript{29+}, W\textsuperscript{39+}, W\textsuperscript{27+}, W\textsuperscript{28+}, and W\textsuperscript{64+} [32–34]. Meng et al and Wu et al also used FAC to calculated data for W\textsuperscript{42+}, and W\textsuperscript{37+}–W\textsuperscript{46+}, respectively [35–37]. More recently, Kwon et al calculated DR rate coefficients for W\textsuperscript{45+} [38]. However, these authors noted that important channels were left out of their calculation. Kwon et al later published an erratum including the updated calculation, as well as the rate coefficients for two additional ions, W\textsuperscript{46+} and W\textsuperscript{44+} [39]. All of these codes are distorted wave. Ballance et al used the dirac atomic R-matrix to calculate DR rate coefficients for W\textsuperscript{35+} [40] to provide a comparison with CA and distorted wave methods.

The Tungsten Project was described by Preval et al., which is a programme of work in which we aim to calculate partial final-state resolved and total zero-densit DR rate coefficients for the entire iononuclear sequence of tungsten. The calculated data from the project is hosted on the Open Atomic Data and Analysis Structure (OPEN-ADAS) website4 in the standard adf09 (DR) and adf48 (RR) formats, the definitions of which can be found on5. As introduced by Preval et al., we use some technical notation when referring to the various ionisation stages of tungsten. As it is not particularly helpful to refer to elements with atomic number Z > 30 by their isoelectronic symbols, we refer to different ionisation states by the number of their valence electrons. In this scheme, H-like (Z = 1) becomes 01-like, Z-like (Z = 30) becomes 30-like, and Pa-like (Z = 46) becomes 46-like, and so on.

In this paper we consider the ionisation stages 19- to 36-like, which covers ions with ground configurations 3d\textsuperscript{q}(q = 1, 10), and 4s\textsuperscript{r}{4p\textsuperscript{t}}(r = 1, 2 and t = 0 – 6). The paper is structured as follows. Section 2 gives a brief overview of the theory used in calculating the DR/RR rate coefficients. In section 3, we discuss the calculations performed for DR and RR, including the configurations used, and the core-excitations considered. In section 4 we discuss the results obtained, and consider the effects of relativistic configuration mixing on the partial and total DR rate coefficients. We make comparisons between our calculated data,
and those mentioned in the previous paragraphs. We also quantify changes to the ionisation balance when using the newly calculated data. We then summarise our results and make some concluding remarks.

2. Theory

The underlying theory of our calculations was discussed at length in Preval et al [13]; however, we provide a brief recap here. The DR rate coefficients were calculated using the distorted-wave collision package AUTOSTRUCTURE [41–43], which uses the independent processes and isolated resonances approximation [44]. AUTOSTRUCTURE has been tested at length by comparing with theory (see Savin et al [45]) and experiment over the past 30 years. The partial DR recombination rate coefficient $\alpha_{j'f}^{z+1}(T_e)$, from initial state $\nu$ of ion $X^{z+}$ to a final state $f$ of ion $X^{z'}$, can be written as

$$
\alpha_{j'f}^{z+1}(T_e) = \frac{4\pi a_0^2 I_H}{k_B T_e} \sum_j \frac{\omega_j}{2\omega_f} \exp \left( -\frac{E}{k_B T_e} \right) \times \sum_n \frac{A_{nj'}^{f} \sigma_{ij'}^{pl}(E)}{A_{n'j'}^{f} \sigma_{ij'}^{pl}(E)}
$$

where the $A_{n}^{\ell}$ are the autoionization rates, $A_{n}^{\ell}$ are the radiative rates, $\omega_{f}$ is the statistical weight of the $N$-electron target ion, $\omega_{f}$ is the statistical weight of the $(N+1)$-electron state, $E$ is the total energy of the continuum electron, minus its rest energy, and with corresponding orbital angular momentum quantum number $l$ labelling said channels. The sum over $j$ represents the sum over all autoionizing states. The sum over $h$ and $m$ represent the total radiative and autoionization widths ($h=1$), respectively. $I_{H}$ is the ionisation energy of the hydrogen atom, $k_B$ is the Boltzmann constant, $T_{e}$ is the electron temperature, and $(4\pi a_0^2)\beta^2 = 6.6011 \times 10^{-24}$ cm$^3$.

While no longer dominant, the RR rate coefficients are still significant, contributing 14% to the total recombination rate coefficient for 19-like. The total recombination rate is necessary to calculate the ionisation balance. Using detailed balance, the partial RR rate coefficient $\alpha_{j'f}^{z+1}(T_e)$ can be written in terms of its inverse process, photoionization $\pi \sigma_{ij'}^{pl}(E)$:

$$
\alpha_{j'f}^{z+1}(T_e) = \frac{c \alpha^3}{\sqrt{\pi}} \frac{\omega_f}{2\omega_f} (I_H k_B T_e)^{-3/2}
\times \int_{0}^{\infty} E_{ij'}^{f} \pi \sigma_{ij'}^{pl}(E) \exp \left( -\frac{E}{k_B T_e} \right) dE,
$$

where $E_{ij'}^{f}$ is the corresponding photon energy and $c \alpha^3/\sqrt{\pi} = 6572.67$ cm s$^{-1}$.

Relativistic corrections to the Maxwell–Boltzmann distribution become important at high temperatures. This correction manifests as a multiplicative factor to give the Maxwell–Jüttner distribution [46] as

$$
F_\ell(\theta) = \frac{\pi \theta}{2} \left( K_2(1/\theta) e^{1/\theta} \right),
$$

where $\theta = \alpha^3 k_B T/2I_H$, $\alpha$ is the fine-structure constant and $K_2$ is the modified Bessel function of the second kind.

3. Calculations

3.1. DR

We split our calculations into core-excitations. These core-excitations are labelled by the initial and final principal quantum numbers $n$ and $n'$ of the promoted target electron. Excitations into the various $\ell$-values associated with $n$ and $n'$ is implied with this notation. The total contribution from inner-shell DR ($n = n' - 1$, $n = 2$) for 19- to 27-like is relatively small, as the full 3s and 3p shells restricts excitations only to 3d. Comparatively, the contribution from inner-shell DR ($n = n' - 1$, $n = 3$) for 29-like onwards is much larger, as there are up to two 3s and six 3p electrons available to promote to 4f. Core-excitations where $\Delta n > 1$ tend to give smaller contributions to the total rate coefficients ($< 10\%$), as DR tends to be suppressed by autoionization into excited states. It is for this reason that we opt to calculate the inner-shell DR ($n = n' - 1$, $n = 2$) and $\Delta n > 1$ core-excitations in CA.

A full list of the core-excitations we calculated DR rate coefficients for is given in table 1. For outer-shell DR, the

| Ion-like Symbol | Core-excitations | Ion-like Symbol | Core-excitations |
|-----------------|------------------|-----------------|------------------|
| W$^{55+}$ $n$-state | 2–3$, n-3$, 3–4, 3–5$ | W$^{38+}$ $n$-state | 3–4, 3–5$ |
| W$^{54+}$ $n$-state | 2–3$, n-3$, 3–4, 3–5$ | W$^{55+}$ $n$-state | 3–4, 4–5, 4–6$ |
| W$^{53+}$ $n$-state | 2–3$, n-3$, 3–4, 3–5$ | W$^{44+}$ $n$-state | 3–4, 4–5, 4–6$ |
| W$^{52+}$ $n$-state | 2–3$, n-3$, 3–4, 3–5$ | W$^{33+}$ $n$-state | 3–4, 4–5, 4–6$ |
| W$^{51+}$ $n$-state | 2–3$, n-3$, 3–4, 3–5$ | W$^{32+}$ $n$-state | 3–4, 4–5, 4–6$ |
| W$^{50+}$ $n$-state | 2–3$, n-3$, 3–4, 3–5$ | W$^{41+}$ $n$-state | 3–4, 4–5, 4–6$ |
| W$^{49+}$ $n$-state | 2–3$, n-3$, 3–4, 3–5$ | W$^{31+}$ $n$-state | 3–4, 4–5, 4–6$ |
| W$^{48+}$ $n$-state | 2–3$, n-3$, 3–4, 3–5$ | W$^{29+}$ $n$-state | 3–4, 4–5, 4–6$ |
| W$^{47+}$ $n$-state | 2–3$, n-3$, 3–4, 3–5$ | W$^{28+}$ $n$-state | 3–4, 4–5, 4–6$ |

Note. Core-excitations marked with an * were calculated only in CA, while the others were calculated in IC.
Table 2. Example of configurations included for DR rate coefficient calculation for the 30-like 4–5 core-excitation.

| \(N\)-electron | \((N+1)\)-electron |
|----------------|------------------|
| \(4s^2\) | \(4s^25s\) |
| \(4s^4p\) | \(4s^4p5p\) |
| \(4s^4d\) | \(4s^4d5d\) |
| \(4s^4f\) | \(4s^4f5f\) |
| \(4s^5s\) | \(4s^5s5g\) |
| \(4s^5p\) | \(4s^5p5s\) |
| \(4s^5d\) | \(4s^5d5d\) |
| \(4s^5f\) | \(4s^5f5f\) |
| \(4p^2\) | \(4p^25g\) |
| \(4p^4d\) | \(4p^4d5s\) |
| \(4p^4s\) | \(4p^4s5p\) |
| \(4p^4d\) | \(4p^4d5d\) |
| \(4p^4f\) | \(4p^4f5f\) |
| \(4p^5s\) | \(4p^5s5s\) |
| \(4p^5p\) | \(4p^5p5p\) |
| \(4p^5d\) | \(4p^5d5d\) |
| \(4p^5f\) | \(4p^5f5f\) |
| \*\(4p^2\) | \(\*4p^25g\) |
| \*\(4p^4d\) | \(\*4p^4d5s\) |
| \*\(4p^4s\) | \(\*4p^4s5p\) |

Note. Configurations marked with an * are included for mixing purposes by way of the one-up, one-down rule.

\(N\)-electron configurations included consist of all possible single-electron promotions from \(nl\) to \(n'\ell'\), where \(n\) and \(n'\) are given by the core-excitation being considered. In addition, configurations accessible by mixing are included. Mixing effects are strongest for terms/levels that are close in energy. The strongest mixing configurations can be determined using a ‘one-up, one-down’ rule. For example, in the \(n=4\) complex, if we have a configuration \(4s^4\mu^\nu^\rho\ell^\mu'\nu'\rho'\ell'\), where \(\mu, \nu, \rho\), and \(\sigma\) are occupation numbers, then the strongest mixing configurations expected would be:

- \(4s^4\mu+14p^\nu+14d^\rho+14f^{\sigma-1}\)
- \(4s^4\mu+14p^\nu-14d^\rho-14f^{\sigma+1}\)
- \(4s^4\mu-14p^\nu+24d^\rho+14f^{\sigma+1}\)
- \(4s^4\mu+14p^\nu-24d^\rho-14f^{\sigma-1}\)
- \(4s^4\mu+14p^\nu-14d^\rho+24f^{\sigma+1}\)
- \(4s^4\mu-14p^\nu+14d^\rho-24f^{\sigma-1}\)

The \((N+1)\)-electron configurations included are simply the \(N\)-electron configurations with an additional target electron added to the final recombined \(n'\ell\) shell. As an example, we give a list of configurations included for the 30-like 4–5 core-excitation calculation in table 2. For inner-shell DR, the configurations included are similar to that of outer-shell DR, except additional core-rearrangement configurations are included. We include an example of the configuration set for 30-like 3–4 in table 3.

Table 3. Example of configurations included for DR rate coefficient calculation for the 30-like 3–4 core-excitation.

| \(N\)-electron | \((N+1)\)-electron |
|----------------|------------------|
| \(3p^63d^{10}4s^2\) | \(3p^63d^{10}4s^24p\) |
| \(3p^63d^{10}4s^4p\) | \(3p^63d^{10}4s^24d\) |
| \(3p^63d^{10}4s^6d\) | \(3p^63d^{10}4s^24f\) |
| \*\(3p^63d^{10}4s^8d\) | \*\(3p^63d^{10}4s^24g\) |
| \*\(3p^63d^{10}4s^10\ell\) | \*\(3p^63d^{10}4s^24n\ell\) |

Note. Configurations marked with an * are included for mixing purposes by way of the one-up, one-down rule. Configurations with 'nf' are the core-rearrangement configurations. For example, the first core-rearrangement configuration is formed by the reaction \(3p^63d^{10}4s^24n\ell\rightarrow 3p^63d^{10}4s^24n\ell + e^-\).

For the Rydberg \(nl\) electron calculation, we calculate radiative/autoionization rates for all individual \(n\) up to \(n=25\), after which they were calculated for logarithmically spaced \(n\) up to \(n=999\). This was done up to \(\ell\)-values such that the total DR rate coefficients for a particular core-excitation are converged numerically to \(<1%\) over the entire ADAS temperature range, given by \((10 - 10^6)z^2\) K, where \(z\) is the residual charge of the target ion.

As one moves deeper into the 3d shell the complexity of the calculation increases dramatically. It quickly becomes necessary to neglect certain subshells and restrict electron promotions when calculating DR rate coefficients in IC. Fortunately, only the 3–4 core-excitation needs to be restricted in this way. For ions 20-like to 33-like promotions from \(3s\rightarrow 4\ell\) can be neglected. For ions 34- to 36-like promotions from \(3s\), \(3p\rightarrow 4\ell\) can be neglected.

We performed calculations in CA to estimate the contributions of promotions from these neglected subshells in IC to the total DR rate coefficient for the 3–4 core-excitation. In the case of 20-like, the \(3s\rightarrow 4f\) promotions contribute 9% to the total 3–4 core-excitation at peak abundance (1.08 \(\times 10^8\) K) for 20-like. Overall, the 3–4 core-excitation contributes 52% to the total recombination rate coefficient, resulting in a 5% difference to the totals upon neglecting the...
Table 4. Example of configurations included for RR rate coefficient calculation for 30-like.

| $N$-electron | $(N + 1)$-electron |
|--------------|-------------------|
| $4s^2$       | $4s^24p$          |
| $4s4p$       | $4s^24d$          |
| $4s4d$       | $4s^24f$          |
| $4s4f$       | $4s^24p^2$        |
| $*4p4d$      | $4s4p4d$          |
| $*4p^2$      | $4s4p4f$          |
|              | $4s^24d^2$        |
|              | $4s4d4f$          |
|              | $4s4f^2$          |
|              | $*4p^24d$         |
|              | $*4p4d4f$         |
|              | $*4p^3$           |
|              | $*4p^24f$         |

Note. Configurations marked with an * are included for mixing purposes by way of the one-up, one-down rule.

3s contribution. The $3s \rightarrow 4\ell$ contribution decreases rapidly as the $3d$, $4s$, and $4\ell$ shells are filled. By 28-like, $3s \rightarrow 4\ell$ promotions contribute 1% to the total at peak abundance. In the case of 33- to 36-like, the $3p$ contribution to the total 3–4 core-excitation for 33-like is just 3% at peak abundance, again decreasing rapidly to <1% by 36-like. For 34-like onwards, we also close the $3p$ shell, considering only $3d - 4\ell$ contributions.

3.2. RR

RR is simpler to calculate in comparison to DR. Preval et al [13] showed that RR was very important at the highest ionisation stages. The set of configurations included mirrored the $\Delta n = 0$ DR configurations for simplicity. In reality, the set of configurations that need to be included in an RR calculation is smaller than this. Including additional configurations increases the computational time, and contributes little to the final result. Therefore, the $N$-electron configurations retained consist of the ground plus single excitations of the outermost electron within the complex. We also include any mixing configurations as given in the previous subsection. The $(N + 1)$-electron configurations are just the $N$-electron configurations with an extra target electron. As an example, we have listed the $N$- and $(N + 1)$-electron configurations included for 30-like in table 4.

RR rate coefficients were calculated for all individual $n$ up to $n = 25$, after which they were calculated for logarithmically spaced $n$ up to $n = 999$. We included $\ell$-values up to $\ell = 10$ relativistically, after which a non-relativistic, hydrogenic ‘top-up’ was included to numerically converge the total to <1% over the entire ADAS temperature range. The RR rate coefficients were calculated in both IC and CA. In the IC case, contributions from multipolar radiation up to E40 and M39 were included, whereas for CA, multipolar radiation contributions up to E40 alone were included.

![Figure 2](image1.png)  
**Figure 2.** DR rate coefficients for each core-excitation of 19-like tungsten, the RR rate coefficient, and the total of these. The parabola is the ionisation fraction for 19-like, calculated using Pütterich et al [12]’s recombination rate coefficients, and Loch et al [14]’s ionisation rate coefficients. The bottom plot gives the cumulative contribution of each recombination rate coefficient, and is described in text.

![Figure 3](image2.png)  
**Figure 3.** The same as figure 2, but for 24-like.

4. DR—results

In this section we describe the DR rate coefficients calculated. We opt to split this section up by the complex being filled, and the core-excitation being considered.

4.1. DR of $3d^q$, $q = 1, 10$

The $3d^q$ ions cover 19-like to 28-like. 28-like, or Ni-like, with a $3d^{10}$ ground state. It is an important ionisation stage where the relatively few strong excitation lines, because of its simplicity, are used in plasma diagnostics. In figures 2 and 3 we have plotted the total DR rate coefficients for 19- and 24-like tungsten along with the cumulative fraction of the individual contributions to the total. The cumulative fraction is calculated by adding successive core-excitations together, starting with the largest, and dividing the result by the total recombination rate coefficient. This allows a quantitative assessment
of which core-excitations are important, and also shows the convergence of the total recombination rate coefficient.

4.1.1. 2–3. The 2–3 core-excitation provides the smallest contribution to the total DR rate coefficient. We include 2–3 for completeness, and calculate this core-excitation in CA only due to its small contribution to the total DR rate coefficient. The 2–3 core-excitation contributes 4% to the total DR rate coefficient for 19-like at peak abundance temperature \( \left(1.2 \times 10^8 \text{K}\right) \), dropping to 0.2% at 27-like. In figure 4 we plot the 2–3 DR rate coefficients for 19- to 27-like calculated in CA. In this plot, a region enclosed by two vertical dashed lines and labelled ‘CP’ (collisionally ionised plasma) indicates the range of peak abundance temperatures from 19-like to 27-like. Note that the actual range of temperatures of interest will be wider than this. It can be seen that the contribution from this core-excitation decreases rapidly as the residual charge decreases, due to the 3d shell being filled.

4.1.2. 3–3. The 3–3 core-excitation provides a large contribution to the total DR rate coefficient at higher charges. Like 2–3, the 3–3 contribution decreases steadily with decreasing residual charge. For 19-like, 3–3 contributes 24% to the total DR rate coefficient at peak abundance, decreasing gradually to 3% by 27-like. In figures 5 and 6 we plot the 3–3 DR rate coefficients for 19- to 27-like in both IC and CA, and indicate the CP range for these ions. There is not much difference between the total 3–3 DR rate coefficients when looking at the CA or IC results. In both cases, the rate coefficients decrease with decreasing residual charge. However, for the IC results, it can be seen that 22- and 23-like swap order, with 23-like becoming larger than 22-like in the CP range. This suggests that 23-like is quite sensitive to relativistic configuration mixing, which is not present in the CA calculation.

4.1.3. 3–4. The 3–4 core-excitation provides by far the largest contribution to the total DR rate coefficient. This is due to the large number of possible transitions that can take place by the six 3p electrons to 4f. The 3–4 core-excitation contributes 51% to the total DR rate coefficient for 19-like, increasing to 79% by 28-like. In figures 7 and 8 we have plotted the 3–4 DR rate coefficients for 19- to 28-like calculated in IC and CA. We have also plotted the CP temperature region for these ions. As with 3–3, the difference between the IC and CA totals are not very different. However, it can be seen that the 3–4 rates span a very narrow range in the CP region regardless of the residual charge. This suggests that the DR rate coefficients for 3–4 are quite insensitive to changes in the atomic structure. This insensitivity also gives an indication of the uncertainty of the calculated DR rate coefficients. Furthermore, there does not appear to be any correlation between the DR rate coefficient and the residual charge. For example, instead of the DR rate coefficient increasing or decreasing in tandem with the residual charge, some rate coefficients are higher than others. There are
resonances close to threshold, and their positioning will cause any variation seen at lower temperatures.

4.1.4. 3–5. Like 2–3, the 3–5 core-excitation has been included for completeness, and has been calculated in CA only due to its small contribution to the total DR rate coefficient. The 3–5 core-excitation contributes 6% at peak abundance for 19-like. As we progress along 19- to 27-like, the 3–5 contribution increases very gradually to 13% by 28-like. In figure 9 we have plotted the 3–5 DR rate coefficients for 19- to 28-like calculated in CA, and have indicated the CP temperature region for these ions. Like 3–4, it can be seen that the 3–5 DR rate coefficients are confined to a narrow band, and do not vary much with respect to ionisation stage. This again indicates that the DR rate coefficients are relatively insensitive to the atomic structure. There are no resonances near threshold.

4.2. DR of 4s[q], q = 1, 2, and 4p[r], r = 1, 6

The 4s[q] ions cover 29-like and 30-like, and the 4s[2]4p[r] ions cover 31-36-like. In figures 10 and 11 we have plotted the DR and RR rate coefficients for 29- and 34-like, along with the cumulative fraction described earlier.
4.2.1. 3–4. The 3–4 core-excitation is an inner-shell process, and remains a significant contributor to the total DR rate coefficient providing 78% at peak abundance temperature for 29-like. This decreases as the $n = 4$ shell is filled, contributing 13% by 36-like at peak abundance. The 3–4 core-excitation remains the dominant contributor to the total recombination rate coefficient until 32-like, giving way to 4–4 and 4–5 at ionisation stages lower than this. In figure 12 we have plotted the 3–4 DR rate coefficients for 29- to 36-like calculated in IC, and have indicated the CP temperature region for these ions. As the $n = 4$ shell fills, the number of possible promotions from $n = 3$ decreases. This leads to a decrease in the DR rate coefficient.

In figure 13 we have plotted the 3–4 DR rate coefficients for 29- to 36-like calculated in CA. By comparing figures 12 and 13, it can be seen that the total DR rate coefficient decreases much faster in the CP region in IC than it does for CA. The suppression effect also becomes much stronger with decreasing residual charge. For 29-like, the CA result is 22% larger than the IC result at peak abundance, whereas for 36-like the CA result is 83% larger than the IC result at peak abundance. This increase in the suppression effect is due to electrons being more tightly bound in the $3d$ shell as the $4s$ and $4p$ shells are filled, further increasing the Auger yield.

4.2.2. 4–4. The 4–4 core-excitation becomes the dominant contribution to the total recombination rate coefficient from 33-like onwards. This is a simple consequence of the $n = 4$ shell filling and suppressing the 3–4 core-excitation. In figure 14 we have plotted the 4–4 total DR rate coefficients for 29- to 36-like calculated in IC, and have also included the CP temperature region for these ions. For 29-like, 4–4 contributes 11% to the total recombination rate coefficient at peak abundance, whereas for 36-like, 4–4 contributes 58%. The total DR rate coefficient jumps noticeably between 29- and 30-like. This is a simple consequence of adding a second electron which effectively doubles the DR rate coefficients of 29-like. A similar jump is seen between 30- and 31-like. The DR rate coefficients are very similar for 31- and 32-like. The DR rate coefficients appear to jump again between 33- and 36-like. In both the 31- to 32-like and 33- to 36-like the DR rate coefficients are confined to a tight band of values. This implies that 33- to 36-like are relatively insensitive to structural changes. With the exception of 36-like, the total DR rate coefficient appears to increase in tandem with a decreasing residual charge at peak abundance temperature. In the case of 36-like, the total DR rate coefficient decreases sufficiently to place it between 33- and 34-like. This is due to the $4p$ shell being completely filled, and preventing $4p - 4p$ transitions occurring.

In figure 15 we plot the DR rate coefficients again but calculated in CA. Similar to figure 14 there is a jump in the total DR rate coefficient between 29- and 30-like, however, the banded structure observed in the IC results is not seen in the CA results. Instead, from 30-like the DR rate coefficient increases steadily with decreasing charge residual. It is also seen that, contrary to the IC results, the DR rate coefficients increase in tandem with a decreasing charge residual at peak abundance temperature, with 36-like being the largest. This is easily explained as the $4p - 4p$ transition cannot occur in CA as it is an elastic transition.

![Figure 12](image1.png)  
Figure 12. Total DR rate coefficients for the 3–4 core-excitation for ionisation stages 29- to 36-like tungsten calculated in IC.

![Figure 13](image2.png)  
Figure 13. The same as figure 12, but calculated in CA.

![Figure 14](image3.png)  
Figure 14. Total DR rate coefficients for the 4–4 core-excitation for ionisation stages 29- to 36-like tungsten calculated in IC.

![Figure 15](image4.png)  
Figure 15. Total DR rate coefficients for the 4–4 core-excitation for ionisation stages 29- to 36-like tungsten calculated in CA.
4.2.3. 4–5. The 4–5 core-excitation is initially comparatively small with respect to 3–4 and 4–4, increasing to be the second largest contribution to the recombination rate total by 36-like. For 29-like, 4–5 contributes 4% at peak abundance. This steadily increases as we move along the charge states, contributing 22% at peak abundance by 36-like. In figure 16 we have plotted the 4–5 DR rate coefficients for 29- to 36-like calculated in IC, and have also indicated the CP temperature region for these ions. As seen in the 4–4 core excitation, there appears to be a banded structure, where a large jump is seen between 29- and 30-like, and between 30- and 31-like. Again, the 31- and 32-like DR rate coefficients are very similar. There is another large jump between 32- and 33-like. Interestingly, in this case, 33-like is not grouped together with 34- to 36-like. Again, as observed in 4–4, the total DR rate coefficients for 36-like

In figure 17 we plot the total DR rate coefficients for 4–5 calculated in CA. 4–5 in CA bears many similarities to 4–4 in CA, in that only a single large jump in DR rate coefficient is seen between 29- and 30-like. In addition, from 30- to 36-like, the DR rate coefficient increases in tandem with decreasing residual charge at peak abundance temperature with 36-like being the largest.

4.2.4. 4–6. The 4–6 core-excitation provides the smallest contribution to the total recombination rate coefficient. It has been included for completeness, and was calculated in CA. For 29-like, 4–6 contributes 0.6% at peak abundance. This increases steadily with decreasing residual charge, contributing 3% by 36-like. In figure 18 we have plotted the 4–6 DR rate coefficients for ionisation stages 29- to 36-like. We have also indicated the CP temperature region for these ions. It can be seen that the rate coefficient spans ~1 dex over 29- to 36-like. As the \( n = 4 \) shell fills, more electrons can be excited to the \( n = 6 \) shell, increasing the DR rate coefficient with decreasing residual charge.

5. RR—results

RR becomes less important to the total recombination rate coefficient as the residual charge decreases. However, RR is not negligible. For the ions considered, the RR rate coefficients are largest for 19-like, contributing 14% to the total recombination rate coefficient. This steadily decreases as the residual charge decreases. At peak abundance temperature, RR contributes 12%, 9%, and 8% to the total recombination rate coefficient.
rate coefficient for 22-like, 25-like, and 28-like, respectively, for the M-Shell. In the N-shell, RR contributes 7% and 4% to the total for 29-like and 36-like, respectively, at peak abundance temperature.

6. Discussion—relativistic configuration mixing

As we move along the isonuclear sequence the atomic structure becomes more complex. With the addition of more electrons, there are more possible ‘one-up, one-down’ configurations. The effect of mixing can be observed by comparing results calculated in IC and CA. However, as mentioned in Preval et al [13], examining the differences between IC and CA using only the totals can be misleading. Therefore, we must look to the partial DR rate coefficients. In figure 19 we have plotted the IC and CA partial DR rate coefficients for 30-like 4–4, where the incident electron recombines into \( n = 4–8 \). At peak abundance temperature, the \( n = 4–8 \) CA partials differ from their IC counterparts by 50% to a factor \(~ 2\). In figure 20 we now plot the partial DR rate coefficients for 30-like 4–5 recombining into \( n = 5–8 \), again in IC and CA. At peak abundance temperature, the \( n = 5–8 \) CA partials differ from their IC counterparts by 50%–70%. Due to the large differences between IC and CA, these results highlight the importance of mixing, and also reinforces the need to use IC results when at all possible.

7. Discussion—comparison with other works

There is little published data for the partial 3d\(^{4}\) DR rate coefficients, possibly because of the complexity of the calculations. However, as mentioned in the Introduction, Meng et al [35] have calculated total DR rate coefficients for 27-like (3d\(^{5}\)) using FAC. 28-like and beyond have multiple datasets available to compare with. Before comparing our results, we sum the DR rate coefficients for all core excitations for the charge-state concerned. Furthermore, we also omit the relativistic Jüttner correction for ease of comparison. In all of our comparisons, the percentage difference between our DR rate coefficients \( \alpha_{0}(T) \) and other authors’ DR rate coefficients \( \alpha_{i}(T) \) at some temperature \( T \) is given as a fraction relative to our data, and is calculated as

\[
\% (T) = 100 \times \frac{\alpha_{i}(T) - \alpha_{0}(T)}{\alpha_{0}(T)}. \tag{4}
\]

7.1. 27-like

The only data available for this ionisation stage was calculated by Meng et al [35]. In table 5 we have tabulated the present DR rate coefficient for 27-like along with Meng et al’s, and the % difference between them. In general, Meng et al’s DR rate coefficients are larger than ours: at the peak abundance temperature (5.97 × 10\(^{6}\) K), they differ from the current work by 31%. The agreement between our and Meng et al’s results (calculated using FAC) provides a benchmark against AUTOSTRUCTURE, and also shows that our calculation is reliable.

7.2. 28-like

28-like is a closed shell ion (3d\(^{10}\)). It is a simple ion in terms of the possible DR channels available, and it is also important in plasma diagnostics, warranting much attention in the modelling community. In figure 21 we have plotted our total DR rate coefficients for 28-like, along with the results of Behar et al [21], Safronova et al [25], Kwon et al [38], and Wu et al [36]. We find that agreement between our DR rate coefficients, Behar et al’s, and Kwon et al’s is generally good at peak abundance temperature (5.1 × 10\(^{7}\) K), differing by 7% and 19%, respectively. However, agreement is much poorer for Safronova et al and Wu et al, differing from our rate coefficients by 27% and 70%, respectively. In all cases, there are large discrepancies exceeding 20% between our data and that of the other four authors at low temperature.
Table 5. Comparison of 27-like total DR rate coefficients between the current work, and Meng et al. [35]. Note [a] = 10^4.

| Temp (K) | This work | Meng | % Diff |
|----------|-----------|------|--------|
| 4.70[+5] | 9.47[−10] | 1.04[−09] | 9.63   |
| 6.37[+5] | 9.05[−10] | 9.70[−10] | 7.14   |
| 8.64[+5] | 8.48[−10] | 8.89[−10] | 4.87   |
| 1.17[+6] | 7.70[−10] | 7.99[−10] | 3.74   |
| 1.59[+6] | 6.75[−10] | 6.99[−10] | 3.50   |
| 2.16[+6] | 5.75[−10] | 5.99[−10] | 4.09   |
| 2.92[+6] | 4.81[−10] | 5.12[−10] | 6.52   |
| 3.97[+6] | 4.00[−10] | 4.43[−10] | 10.8   |
| 5.38[+6] | 3.36[−10] | 3.89[−10] | 15.8   |
| 7.30[+6] | 2.85[−10] | 3.44[−10] | 20.7   |
| 9.90[+6] | 2.39[−10] | 2.98[−10] | 24.7   |
| 1.34[+7] | 1.95[−10] | 2.49[−10] | 27.6   |
| 1.82[+7] | 1.53[−10] | 1.98[−10] | 29.2   |
| 2.47[+7] | 1.16[−10] | 1.51[−10] | 29.9   |
| 3.35[+7] | 8.44[−11] | 1.10[−10] | 30.4   |
| 4.54[+7] | 5.94[−11] | 7.77[−11] | 30.7   |
| 6.16[+7] | 4.08[−11] | 5.34[−11] | 31.1   |
| 8.35[+7] | 2.74[−11] | 3.60[−11] | 31.3   |
| 1.13[+8] | 1.82[−11] | 2.39[−11] | 31.2   |
| 1.54[+8] | 1.19[−11] | 1.56[−11] | 31.0   |
| 2.08[+8] | 7.78[−12] | 1.02[−11] | 30.6   |
| 2.83[+8] | 5.03[−12] | 6.55[−12] | 30.3   |
| 3.83[+8] | 3.23[−12] | 4.21[−12] | 30.2   |
| 5.20[+8] | 2.07[−12] | 2.69[−12] | 30.4   |
| 7.05[+8] | 1.31[−12] | 1.72[−12] | 30.9   |

Figure 21. Total DR rate coefficients of 28-like as calculated in this work (black solid), Behar et al. [21] (red dotted), Safronova et al. [28] (blue dash), Kwon et al. [39] (green dashed–dotted), and Wu et al. [36] (cyan triple dotted–dashed).

The difference increases to a factor 16. Towards higher temperatures (~1 × 10^5 K). However, these variations occur well outside relevant plasma temperatures. Such variations are likely caused by the positioning of low temperature DR resonances, which are present in our calculation. The good agreement between Behar et al., Kwon et al., and our results show that the calculations are reliable. In the case of the outliers, this gives an idea of the uncertainty in the calculation of the total DR rate coefficients.

7.3. 29-like

In figure 22 we have plotted the total DR rate coefficients for 29-like from this work, Safronova et al. [27] (using HULLAC), Kwon et al. [38], and Wu et al. [36] (both using FAC). Prior to the present work, there was no consensus between calculations. Good agreement is seen between our data and Kwon’s at peak abundance temperature (4.32 × 10^5 K) differing by 23%. Interestingly, we see even better agreement between our rate coefficients and Kwon’s at lower temperatures (~1 × 10^5 K), with the difference being 2% in places. However, from temperatures exceeding 4.5 × 10^5 K, the difference gradually increases, reaching 26% by 1 × 10^6 K, where the rate coefficient is falling off rapidly.

Figure 22. Total DR rate coefficients of 29-like tungsten as calculated in this work (black solid), Safronova et al. [27] (blue dash), Kwon et al. [39] (green dashed–dotted), and Wu et al. [36] (cyan triple dotted–dashed).

Figure 23. Total DR rate coefficients of 30-like tungsten as calculated in this work (solid line), Kwon et al. [39] (green dashed–dotted), and Wu et al. [36] (cyan triple dotted–dashed).
temperatures where $T^{-3/2}$ behaviour dominates, the difference stabilises to a factor 9. The size and consistency of this discrepancy implies that there is a systematic uncertainty in Safronova et al’s rate coefficients which is difficult to account for.

We note that discrepancies of the size observed are not limited to this particular ion. For example, in our previous work [13], we noted a discrepancy of 47% between our total DR rate coefficients and that of Safronova et al [30] for 10-like tungsten at high temperatures, but good agreement with the calculations of Behar et al [22], differing from our results by <10%.

In the case of Wu et al, even larger discrepancies are seen. While at low temperatures the agreement is better than 10%, the difference between our and Wu’s data increases gradually to a factor $\sim 4$ at the highest temperatures compared. The difference at peak abundance temperature is a factor 3.7. We defer discussion of this discrepancy to section 7.6.

7.4. 30-like

In figure 23 we have plotted the total DR rate coefficients for 30-like from this work, Kwon et al [38], and Wu et al [36]. As with 29-like, good agreement is seen between our total DR rate coefficients and Kwon et al’s over the entire temperature range considered. At peak abundance temperature ($3.7 \times 10^5$ K) Kwon et al’s DR rate coefficients differ from ours by 14%. Excellent agreement is seen towards lower temperatures, decreasing steadily to 0.5% by $\sim 1 \times 10^5$ K. Towards higher temperatures, the agreement deteriorates slightly, reaching 18% by $\sim 1 \times 10^6$ K.

In the case of Wu et al’s results, agreement is markedly better for 30-like than it was for 29-like. At peak abundance temperature the difference between our and Wu et al’s DR rate coefficients is 43%. Towards lower temperatures this difference increases to 49% before decreasing to 14% at $\sim 1 \times 10^5$ K. Towards higher temperatures, the agreement deteriorates further, reaching 55% by $\sim 1 \times 10^6$ K.

7.5. 31–36-like

In table 6 we list the % difference between our and Wu et al’s total DR rate coefficients over a range of temperatures. Agreement between our and Wu et al’s varies, however, agreement appears to be worse generally at the extremes of low and high temperature. In the case of 31-like, there is generally good agreement at low temperature, where our and Wu et al’s data differ by 10% between $1.2 \times 10^5$ and $4.2 \times 10^6$ K. Beyond $2.7 \times 10^6$ K, our DR rate coefficients gradually become smaller, differing by 88% at peak abundance temperature from Wu et al. Similar differences occur for the following charge states. In figure 24 we plot an example of this for 32-like. At peak abundance temperature, our and Wu et al’s total DR rate coefficients differ by factors of 1.6–2.4 for 32-, 33-, 35-, and 36-like.

In addition to the Wu et al data for 35-like, Li et al has also calculated DR rate coefficients for this ionisation stage. In figure 25 we have plotted our 35-like total DR rate coefficients, and the corresponding DR rate coefficients of Li et al and Wu et al. It can be immediately seen that the size and shape of Li et al’s and Wu et al’s total DR rate coefficients are strikingly similar, differing at most by 7% at $5.6 \times 10^5$ K implying a similar methodology in their FAC calculations. Towards lower temperatures our DR rate coefficients are larger than Li’s differing by 61% at $\sim 1 \times 10^5$ K. Towards higher temperatures the differences are much larger, differing by a factor $\sim 2.5$ at $\sim 1 \times 10^8$ K. At peak abundance temperature ($2.9 \times 10^7$ K) the difference between our data and Li’s is a factor $\sim 2$.

7.6. Auger supression

When comparing our total DR rate coefficients with Wu et al for 29-like to 36-like, we saw that Wu et al’s rate coefficients were consistently larger than ours by significant amounts at low and high temperatures. Kwon et al [39] noted this difference, and attributed the low temperature differences to Wu et al using a simplified set of configurations in their calculations. We do not discuss the low temperature regime further. At high temperatures, Auger suppression effects arising from core rearrangement for inner-shell DR become important. The inclusion of these core-rearrangement configurations is computationally demanding. If core-rearrangement is neglected in inner-shell calculations, the resultant DR rate will be artificially inflated. For 35-like, Wu et al has plotted the 3s-, 3p-, and 3d–n contributions to the total DR rate coefficient (see figure 6 in [36]). In an attempt to explain the discrepancy between our and Wu et al’s results, we repeated our 3–4 core-excitation calculation with the same structure as before, but neglect core-rearrangement. This also partially removes the contribution from radiation into auto-ionizing states. As our 3–4 calculation includes only excitations from 3d, we only compare Wu’s 3d contribution. In figure 26 we plot our 3d–n DR rate coefficients calculated with and without core rearrangement and compare them to Wu’s 3d – n contributions. It can be seen that our non-suppressed calculation is much closer to the Wu result than the suppressed calculation. At peak abundance temperature, the DR rate coefficients including core rearrangement differs from Wu et al’s by a factor $\sim 3$, whereas excluding the core rearrangement decreases this difference to 87%. The remaining difference may come from other core-excitation such as 3–5, 3–6, and so on.

8. Discussion—comparison with Pütterich et al

Agreement between our recombination rate totals and Pütterich et al’s [12] is very good from 19- to 26-like. Recall that Pütterich et al scaled their recombination rate coefficients by empirically determined scaling factors to improve agreement with observed spectral emission. In figure 27 we have plotted the present recombination rate coefficients and Pütterich et al’s scaled and unscaled results for 19-like. We have also included our individual DR and RR contributions to the total. At peak abundance temperature the present recombination rate coefficients for 19-like differ from Pütterich et al’s scaled data by 9%.
Table 6. Table of differences between the total DR rate coefficients as calculated in this work, and by Wu et al [36]. The % difference between the two DR rate coefficients is given relative to the current work. Note $[x] = 10^x$.

| Temp (K) | % Diff 31 | % Diff 32 | % Diff 33 | % Diff 35 | % Diff 36 |
|---------|-----------|-----------|-----------|-----------|-----------|
| 5.80[+4] | 13.2      | -38.3     | -51.1     | -63.2     | -64.4     |
| 8.71[+4] | 16.2      | -36.1     | -50.1     | -61.4     | -56.0     |
| 1.31[+5] | 7.70      | -36.7     | -49.1     | -60.5     | -48.2     |
| 1.96[+5] | 0.23      | -36.5     | -47.5     | -58.3     | -42.1     |
| 2.95[+5] | -3.11     | -35.9     | -45.9     | -53.5     | -37.5     |
| 4.43[+5] | -4.88     | -35.4     | -45.0     | -46.0     | -32.3     |
| 6.65[+5] | -5.90     | -35.9     | -45.5     | -36.9     | -25.9     |
| 9.98[+5] | -6.23     | -37.2     | -46.5     | -28.5     | -18.8     |
| 1.50[+6] | -5.95     | -37.4     | -45.8     | -21.5     | -11.1     |
| 2.25[+6] | -2.66     | -35.2     | -41.9     | -13.4     | -0.75     |
| 3.38[+6] | 4.54      | -29.4     | -33.8     | -2.48     | 13.4      |
| 5.07[+6] | 15.2      | -18.6     | -21.2     | 12.8      | 32.2      |
| 7.62[+6] | 30.6      | -2.43     | -5.09     | 33.1      | 56.1      |
| 1.14[+7] | 49.1      | 17.3      | 12.3      | 57.1      | 83.6      |
| 1.72[+7] | 66.5      | 37.0      | 28.5      | 81.6      | 110       |
| 2.58[+7] | 80.4      | 53.9      | 42.5      | 104       | 133       |
| 3.87[+7] | 90.6      | 67.1      | 53.5      | 121       | 152       |
| 5.81[+7] | 98.5      | 76.9      | 61.7      | 135       | 166       |
| 8.73[+7] | 104       | 84.2      | 67.4      | 145       | 178       |
| 1.31[+8] | 107       | 89.8      | 71.2      | 152       | 186       |
| 1.97[+8] | 109       | 93.7      | 73.7      | 157       | 190       |
| 2.95[+8] | 111       | 95.7      | 75.3      | 160       | 192       |
| 4.44[+8] | 112       | 96.9      | 76.6      | 162       | 195       |
| 6.66[+8] | 113       | 97.8      | 77.7      | 164       | 197       |
| 1.00[+9] | 113       | 98.7      | 78.2      | 165       | 199       |

Figure 24. Total DR rate coefficients of 32-like tungsten as calculated in this work (black solid), and Wu et al [36] (cyan triple dotted–dashed).

The unscaled data for 19-like bears a similar level of agreement with our results, differing by 12% at peak abundance temperature. Similarly, for 24- and 26-like, the differences are 29% and 13%, respectively, for the scaled data. For the unscaled data, the differences are 31% and 45%, respectively.

Beyond 26-like, the agreement between ours and Pütterich et al’s scaled data deteriorates sharply. In figure 28 we have plotted the present recombination rate coefficients and Pütterich et al’s scaled and unscaled results for 27-like, again including the present DR and RR contributions. At peak abundance temperature, our and Pütterich et al’s scaled data differ by a factor $\sim 3$. Interestingly, the unscaled data is in better agreement with our results, where the difference is 57% at peak abundance temperature. For 28-like, the scaled data agrees better than the unscaled data, differing with our results by 29% and 81%, respectively. From 32-like onwards the unscaled data agrees better with our results than the scaled data. However, it should be stressed that while agreement is improved, the difference between our results and the unscaled data is still very large, being 49% for 32-like, increasing to a factor $\sim 2$ for 36-like.
9. Discussion—zero density Ionisation balance

Using our recombination rate coefficients, we calculate the ionisation balance to quantify any changes that occur. To calculate the ionisation fraction, we replace the relevant recombination rate coefficients from Pütterich et al [12] with our data. We use this recombination data in conjunction with the ionisation rate coefficients of Loch et al [14].

In figure 29 we have plotted the ionisation fraction using only the Pütterich et al recombination data, and the ionisation fraction including our data. We have also plotted the difference between the two fractions, which is calculated by subtracting our ionisation fraction from Pütterich et al’s for each charge state. Both ionisation fractions use Loch’s ionisation rate coefficient data. Note that we have removed the Jüttner relativistic correction from our recombination rate coefficients to simplify comparisons. It can be seen that the two ionisation fractions are quite similar up to 27-like. However, for 28-like, we see a significant difference in the position and height of the ionisation fraction. This is caused by the large differences in our and Pütterich et al’s recombination rate coefficients discussed in the previous section. To show this, we have replotted the ionisation fraction in figure 29, but include our data only up to 26-like. It can now be seen that the large difference between the ionisation fractions has now disappeared.

Including our new data up to 36-like has significantly altered the peak abundances and the peak abundance temperatures. In table 7 we have listed the peak abundances and temperatures as calculated when using Pütterich et al’s and our ionisation fractions for 01-like to 36-like. Most notable are the changes to the peak abundance for 28-like, which as
This work with 01- to 36-like replaced with our data. The ionisation rate coefficients originate from Loch et al [14]. Note |x| = 10^x. The peak temperature only changes by <2% from Pütterich et al. to the current work, the fractional abundance drops by 88% from 0.35 to 0.19. The largest peak temperature change occurs for 25-like, decreasing by 13% from 7.4 x 10^7 to 6.6 x 10^7 K. Overall, there does not appear to be a particular trend dictating whether a temperature or fraction will increase or decrease. Furthermore, these temperatures and fractions have been determined in the zero density approximation. The true effect of these changes will only be seen with CR modelling.

10. Conclusions

We have compared our DR rate coefficients with multiple authors. Multiple datasets were available for 28-like, which is mentioned previously, is an important ion in plasma diagnostics.

### Table 7. Comparison of peak abundance temperatures and fractions as calculated using Pütterich et al's data [12], and Pütterich et al's data with 01- to 36-like replaced with our data. The ionisation rate coefficients originate from Loch et al [14]. Note |x| = 10^x.

| Ion-like | Charge | Putt. T_{peak} | Putt. f_{peak} | This work T_{peak} | This work f_{peak} | ΔT%  | Δf% |
|----------|--------|----------------|----------------|-------------------|-------------------|------|----|
| 01-like  | W^{73+} | 3.88 [+9]       | 0.440          | 4.06 [+9]         | 0.426             | −4.50 | 3.14 |
| 02-like  | W^{72+} | 2.29 [+9]       | 0.442          | 2.46 [+9]         | 0.405             | −7.11 | 9.16 |
| 03-like  | W^{71+} | 1.48 [+9]       | 0.360          | 1.64 [+9]         | 0.363             | −10.1 | −0.93 |
| 04-like  | W^{70+} | 9.66 [+8]       | 0.294          | 1.06 [+9]         | 0.304             | −8.84 | −3.30 |
| 05-like  | W^{69+} | 7.17 [+8]       | 0.247          | 7.67 [+8]         | 0.255             | −6.52 | −3.19 |
| 06-like  | W^{68+} | 5.72 [+8]       | 0.218          | 5.97 [+8]         | 0.228             | −4.19 | −4.17 |
| 07-like  | W^{67+} | 4.76 [+8]       | 0.199          | 4.84 [+8]         | 0.213             | −1.61 | −6.28 |
| 08-like  | W^{66+} | 4.03 [+8]       | 0.189          | 3.98 [+8]         | 0.209             | 1.36  | −9.33 |
| 09-like  | W^{65+} | 3.46 [+8]       | 0.195          | 3.32 [+8]         | 0.217             | 3.94  | −9.99 |
| 10-like  | W^{64+} | 2.99 [+8]       | 0.214          | 2.82 [+8]         | 0.229             | 6.25  | −6.57 |
| 11-like  | W^{63+} | 2.60 [+8]       | 0.202          | 2.43 [+8]         | 0.198             | 7.04  | 1.78 |
| 12-like  | W^{62+} | 2.25 [+8]       | 0.188          | 2.11 [+8]         | 0.179             | 6.48  | 5.25 |
| 13-like  | W^{61+} | 2.01 [+8]       | 0.182          | 1.89 [+8]         | 0.174             | 6.19  | 4.53 |
| 14-like  | W^{60+} | 1.80 [+8]       | 0.172          | 1.70 [+8]         | 0.171             | 6.25  | 1.01 |
| 15-like  | W^{59+} | 1.62 [+8]       | 0.163          | 1.52 [+8]         | 0.166             | 6.50  | −1.35 |
| 16-like  | W^{58+} | 1.47 [+8]       | 0.157          | 1.38 [+8]         | 0.167             | 6.74  | −6.02 |
| 17-like  | W^{57+} | 1.36 [+8]       | 0.139          | 1.27 [+8]         | 0.154             | 7.02  | −9.48 |
| 18-like  | W^{56+} | 1.26 [+8]       | 0.140          | 1.16 [+8]         | 0.157             | 7.99  | −10.8 |
| 19-like  | W^{55+} | 1.17 [+8]       | 0.147          | 1.07 [+8]         | 0.150             | 8.96  | −1.73 |
| 20-like  | W^{54+} | 1.08 [+8]       | 0.150          | 9.83 [+7]         | 0.160             | 10.2  | −6.24 |
| 21-like  | W^{53+} | 1.01 [+8]       | 0.148          | 9.01 [+7]         | 0.162             | 11.6  | −9.00 |
| 22-like  | W^{52+} | 9.29 [+7]       | 0.144          | 8.33 [+7]         | 0.167             | 11.6  | −13.6 |
| 23-like  | W^{51+} | 8.60 [+7]       | 0.143          | 7.73 [+7]         | 0.153             | 11.3  | −6.36 |
| 24-like  | W^{50+} | 8.01 [+7]       | 0.146          | 7.14 [+7]         | 0.156             | 12.2  | −5.99 |
| 25-like  | W^{49+} | 7.41 [+7]       | 0.159          | 6.57 [+7]         | 0.164             | 12.7  | −2.96 |
| 26-like  | W^{48+} | 6.74 [+7]       | 0.181          | 6.02 [+7]         | 0.174             | 12.1  | 4.26 |
| 27-like  | W^{47+} | 5.97 [+7]       | 0.136          | 5.47 [+7]         | 0.182             | 9.14  | −25.2 |
| 28-like  | W^{46+} | 5.10 [+7]       | 0.353          | 5.03 [+7]         | 0.188             | 1.45  | 88.0 |
| 29-like  | W^{45+} | 4.32 [+7]       | 0.227          | 4.62 [+7]         | 0.157             | −6.68 | 43.9 |
| 30-like  | W^{44+} | 3.74 [+7]       | 0.196          | 4.21 [+7]         | 0.150             | −11.2 | 30.8 |
| 31-like  | W^{43+} | 3.40 [+7]       | 0.194          | 3.80 [+7]         | 0.177             | −10.4 | 10.1 |
| 32-like  | W^{42+} | 3.22 [+7]       | 0.108          | 3.34 [+7]         | 0.244             | −3.56 | −55.8 |
| 33-like  | W^{41+} | 3.11 [+7]       | 0.044          | 3.06 [+7]         | 0.210             | 1.64  | −79.1 |
| 34-like  | W^{40+} | 3.01 [+7]       | 0.052          | 2.84 [+7]         | 0.149             | 5.80  | −65.2 |
| 35-like  | W^{39+} | 2.91 [+7]       | 0.049          | 2.67 [+7]         | 0.108             | 9.18  | −54.6 |
| 36-like  | W^{38+} | 2.81 [+7]       | 0.093          | 2.52 [+7]         | 0.104             | 11.4  | −10.3 |

Figure 30. The same as figure 29, but including our recombination data up to 26-like only.

Note: D x [x] x et al. = D x [x] x et al. x x et al. x x et al.
an important ion in plasma diagnostics. At peak abundance temperature, our DR rate coefficients agree well with Behar et al [21] and Kwon et al [39], better than 20%. Good agreement with Kwon et al is also seen in 29-like and 30-like, differing from our calculations by ~20%, respectively. In contrast, consistently poor agreement is observed between our data and Wu et al’s [36] for 28-like to 33-like and 35-like to 36-like, with differences sometimes exceeding a factor ~4. This includes ions for which we are in good agreement with Kwon et al. It was found that agreement with Wu et al’s 35-like results could be improved if core-rearrangement suppression was neglected from our inner-shell DR calculations.

We have assessed the effect of relativistic configuration mixing on partial DR rate coefficients in n for 30-like tungsten. This was done by comparing partial DR rate coefficients calculated in IC and CA. It was shown that the largest difference between the two sets of DR rate coefficients at peak abundance temperature was a factor ~2. This is a consequence of the increasing complexity in atomic structure as we move along the isonuclear sequence. The increase in electrons available to promote increases the number of one-up, one-down mixing configurations, hence increasing its importance. This result highlights the importance of using IC DR results where ever possible.

For the purpose of calculating ionisation fractions, we have also calculated the RR rate coefficients alongside the DR rate coefficients in IC and CA. In IC, we included multipolar radiation contributions up to E40 and M39, whereas for CA we only include multipolar contributions up to E40. For 19-like, the RR rate coefficients were found to contribute 14% to the recombination rate total at peak abundance temperature. This contribution decreases steadily with decreasing residual charge to 4% by 36-like.

Comparison of our recombination rate coefficients with the scaled data of Pütterich et al yielded relatively good agreement for ions 19- to 26-like. Beyond 26-like we saw this agreement deteriorate rapidly as we moved along the charge states. We also saw that agreement beyond 26-like was better when comparing our recombination rate coefficients with Pütterich et al’s unscaled data. However, the difference between our and Pütterich et al’s data still exceeded 40%. The large disagreement is to be expected due to the complexity of the ions being considered.

We have presented our DR rate coefficient calculations for ions W55+ to W38+. bringing us halfway into the ions required to calculate the isonuclear sequence of tungsten. Unlike W55+ to W38+ considered in Preval et al [13], the ions considered in this paper will be easily formed in ITER plasma conditions. Our next installment in The Tungsten Project will cover the 4d[n](q = 1 – 10) ions. We split the project in this way in anticipation of covering the 4f-shell ions following our 4d[n] work.

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