Dielectronic Recombination of $W^{45+}$ and $W^{44+}$: Configuration Mixing and Channels

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DR cross sections and rate coefficients have been calculated for W$^{45+}$ and W$^{44+}$ based on an IPIR-DW approximation using flexible atom code (fac).

Effects of configuration mixing (CM) involving double electron core excitation and non-resonant stabilizations + decay to autoionizing levels possibly followed by cascades (DAC) on DR are investigated.
Experimental data is available only for these ions.
Introduction

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DR cross section and rate coefficient

$$e^- + A_i^{q^+} \leftrightarrow [A_j^{(q-1)+}]^{**} \rightarrow [A_f^{(q-1)+}]^* + h\nu.$$  

$$\bar{\sigma}_{ij} = \frac{\pi^2}{E_{ij} \Delta E} \frac{g_j}{2g_i} A_{ji}^a \frac{\sum_t A_{jt}^r + \sum_{t'} A_{jt'}^r B_{t'}}{\sum_k A_{jk}^a + \sum_f A_{jf}^r},$$

$$\bar{\sigma}_{ij}^{DC} = \frac{\pi^2}{E_{ij} 2g_i} A_{ji}^a \frac{\Gamma_j/2\pi}{(E - E_{ij})^2 + \Gamma_j^2/4} \approx \frac{\pi^2}{E_{ij} 2g_i} \frac{g_j}{2g_i} A_{ji}^a \delta(E - E_{ij}).$$

$$\Gamma_j = \sum_k A_{jk}^a + \sum_f A_{jj}^r$$

$$\alpha_{ij}(T_e) = \frac{1}{\pi^{1/2}} \left( \frac{2}{k_B T_e} \right)^{3/2} \int_0^\infty \sigma_{ij}(E) \exp \left( -\frac{E}{k_B T_e} \right) dE$$

$$\approx \frac{1}{2g_i} \left( \frac{4\pi a_0^2 Ry}{k_B T_e} \right)^{3/2} g_j A_{ji}^a B_j \exp \left( -\frac{E_{ij}}{k_B T_e} \right).$$
Calculated energies for $W^{45+}$ and $W^{44+}$

<table>
<thead>
<tr>
<th>Term</th>
<th>Present</th>
<th>NIST % Diff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$3d^{10}4s^2 , ^2S_{1/2}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$3d^{10}4p_2 , ^2P_{1/2}$</td>
<td>97.529</td>
<td>97.626</td>
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<tr>
<td>$3d^{10}4p_2 , ^2P_{3/2}$</td>
<td>198.930</td>
<td>198.897</td>
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<tr>
<td>$3d^{10}4d , ^2D_{3/2}$</td>
<td>349.326</td>
<td>349.59</td>
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<tr>
<td>$3d^{10}4d , ^2D_{5/2}$</td>
<td>370.857</td>
<td>371.153</td>
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<tr>
<td>$3d^{10}4f , ^2F_{5/2}$</td>
<td>532.304</td>
<td>532.31</td>
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<tr>
<td>$3d^{10}4f , ^2F_{7/2}$</td>
<td>537.749</td>
<td>537.74</td>
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<tr>
<td>$3d^{10}5s , ^2S_{1/2}$</td>
<td>967.7</td>
<td>967.6</td>
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<tr>
<td>$3d^{10}5p , ^2P_{1/2}$</td>
<td>1015.1</td>
<td>1014.9</td>
</tr>
<tr>
<td>$3d^{10}5d , ^2D_{3/2}$</td>
<td>1134.4</td>
<td>1136.2</td>
</tr>
<tr>
<td>$3d^{10}5f , ^2F_{5/2}$</td>
<td>1216.4</td>
<td>1216.7</td>
</tr>
<tr>
<td>$3d^{10}5g , ^2G_{7/2}$</td>
<td>1256.4</td>
<td>1256.1</td>
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<tr>
<td>$3d^{10}6f , ^2F_{5/2}$</td>
<td>1586.7</td>
<td>1587.4</td>
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<tr>
<td>$3d^{10}6g , ^2G_{7/2}$</td>
<td>1609.5</td>
<td>1609.4</td>
</tr>
<tr>
<td>$3d^{2}4s^2 , ^2D_{5/2}$</td>
<td>1554.0</td>
<td>1547.6</td>
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<tr>
<td>$3d^{2}2D_{3/2}(4s_{1/2}4P_{1/2})_1$</td>
<td>1713.6</td>
<td>1707.3</td>
</tr>
<tr>
<td>$3d^{2}2D_{3/2}(4p_{1/2})_1$</td>
<td>1816.6</td>
<td>1809.7</td>
</tr>
<tr>
<td>$3p^23d^{10}4s^2 , ^2P_{3/2}$</td>
<td>2010.0</td>
<td>2000.1</td>
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<tr>
<td>$3p^23d^{10}4s^2 , ^2P_{1/2}$</td>
<td>2090.0</td>
<td>2092.2</td>
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<tr>
<td>$3d^{10}4s(5/2, 1/2) 4f_{7/2}$</td>
<td>2090.0</td>
<td>2095.5</td>
</tr>
<tr>
<td>$3p^2(2P_{1/2})3d^{10}(4s_{1/2}4d_{5/2})_3$</td>
<td>2380.0</td>
<td>2367.1</td>
</tr>
</tbody>
</table>

Excellent agreement with the recommended NIST data (0.001 ~ 0.5 %)

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$W^{45+} : 3d + e^- \rightarrow 4l4l' \ (CM \ & NRS + DAC)$

$3s^2 3p^5 3d^{10} 4s + e^- \rightarrow 3d^9 4l4l'n'' \rightarrow \begin{cases} 3d^{10}4l \\ 3d^{10}n''(n > 4) \\ 3d^94l4l'(n > 4) \end{cases} + e^-$

$\rightarrow \begin{cases} 3d^{10}4l4l' \\ 3d^{10}4l'n''(n > 4) \end{cases} + \omega$

Convolved cross section ($10^{-18} \text{ cm}^2$)

Energy (eV)
$W^{45+} : 3d + e^- \rightarrow 4l4l' \ (CM \ & \ NRS+DAC)$
$^{45+} W : 3p + e^- \rightarrow 4l4l' \ (CM \ & \ NRS+DAC)$

\[ 3s^23p^63d^{10}4s + e^- \rightarrow 3p^53d^{10}4l4l'nl'' \rightarrow \begin{cases} 3d^{10}4l \\ 3d^{10}nl''(n > 4) \\ 3d^94l4l' \\ 3p^53d^{10}4l4l'(n > 4) \end{cases} + e^- \]

\[ \rightarrow \begin{cases} 3d^{10}4l4l''(n > 4) \\ 3d^94l4l'n''(n = 4) \end{cases} + \omega \]
$W^{45+} : 3p + e^- \rightarrow 4l4l' \ (CM \ & \ NRS+DAC)$
W^{45+} : 3d → 4l core excitation rate coeff.
$^{45+}_W : 3p \rightarrow 4l$ core excitation rate coeff.

$3p^6 3d^{10} 4s + e^- \rightarrow 3p^5 3d^{10} 4l'i'n'l''$

Rate coefficient (cm$^3$/s)

Energy (eV)
$W^{45+} : 4s \rightarrow 4l$ core excitation

\[ 3s^2 3p^6 3d^{10} 4s + e^- \rightarrow 3d^{10} 4lnl' \rightarrow 3d^{10} 4l + e^- \]

\[ \rightarrow 3d^{10} 4l4l' + \omega \]

![Graph showing rate coefficient vs energy for different values of n from 8 to 500](image)
W^{45+} : 4s → 5l core excitation

\[ 3s^23p^63d^{10}4s + e^- \rightarrow 3d^{10}5lnl' \rightarrow \begin{cases} 
3d^{10}4l \\
3d^{10}5l(n \geq 10)
\end{cases} + e^- \\
\rightarrow \begin{cases} 
3d^{10}4l5l' \\
3d^{10}5l5l' \\
3d^{10}4lnl''(n > 5)
\end{cases} + \omega \]
$W^{45+}$ : Total Rate Coefficient

Submitted.

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\( W^{45+} : \text{Total Rate Coefficient} \)
Resonance profile (dense states)

\[
\sigma_{ij}^{\text{DC}} = \frac{\pi^2}{E_{ij} 2g_i} \frac{\Gamma_j / 2\pi}{(E - E_{ij})^2 + \Gamma_j^2/4} \approx \frac{\pi^2}{E_{ij} 2g_i} A_{ji}^a \delta(E - E_{ij}).
\]

\[
\Gamma_j = \sum_k A_{jk}^a + \sum_f A_{jj}^r
\]

\[
\Gamma_j \rightarrow \Gamma_{sp} = 10 \text{ eV}
\]

Recombination of W\textsuperscript{18+} Ions with Electrons: …

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W^{45+}: Resonance profile (dense states)
$W^{44+} : 4s \rightarrow 4l$ core excitation

Rate coefficient (cm$^3$/s)

Energy (eV)

$3d^{10}4s^2 + e^- \rightarrow 3d^{10}4l\ell'$

$3d^{10}4s^2 + e^- \rightarrow 3d^{10}4s4\ell'$

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DR computation challenges

- Long running time for branching ratio calculation due to so many resonance levels or NRS+DAC consideration as more CM is considered or ion stage with complex configuration structure is treated.

- Parallel algorithms are needed for the AI or RD transition rate calculation.
Our calculated energies for W^{45+} and W^{44+} are in excellent agreement with the recommended NIST data. (0.001 ~ 0.5 %)

CM affects on DR rate coefficient significantly specially at low energies near threshold due to appearance of new resonances or resonance energy shift.

Accurate DR rate coefficient of W^{45+} counting all contributable resonances was provided.

Density effect, GCR and state resolved DR are our future works.