Fundamental atomic data for tungsten and hydrogen and the effect of the finite density edge plasma

Martin O’Mullane, Nigel Badnell, Stuart Henderson, Simon Preval and ADAS contributors
ADAS perspective: wish for complete data for all elements

Equilibrium balance
- rate coefficients for ionisation balance (adf11)
- influx S/XB measure (adf15)
- Radiated power (adf11)
- Spectroscopy (adf15)
- All fundamental atomic data calculated by ADAS group and close collaborators (adf04, adf09, adf48, adf23)

![Graph showing fractional abundances of different elements (H, Be, Ar, Fe, W) as a function of temperature (Te) in keV.](image)

- divertor radiation
- far SOL
- influx
- turbulent transport
- edge transport barrier
- plasma core
- neoclassical accumulation
- radiative mantle
- pedestal
What is an edge ion?

- With increasing Z
  - more and more ion stages exist in a small spatial region
  - individual emission shells become narrow which limits the contribution function of a line
  - more electrons generally complicates the atomic structure spreading emission across many transitions
Fundamental rates alone are not sufficient

- Simple equilibrium balance – no thermal CX or molecular processes.
- Variation with density is possibly greater than any uncertainty in atomic data – particularly for hydrogen.
Opacity effects

- The change is of same order as density variation.
- Demands high precision of the underlying atomic data.
- And correctness of the CR model.

- ADAS generalized collisional-radiative model
- Transition probabilities of Lyman-α reduced to 10% and Lyman-β to 55%.
- Not as extreme as astrophysical Case A.
- Consistent ionization and recombination rates calculated.
New neutral hydrogen excitation data

- 1958 – first measurement of $2p \rightarrow$ ground (Fite and Brackmann).
- 1963 – close coupling calculation (Burke).
- 2020 – $R$-matrix up to $n=8$.
- hydrogen may never be ‘done’.
New excitation data – n=1-5 only

- ADAS generalized collisional-radiative model
- Have not used higher-n to modify high n-n’ transitions so the effect may be greater.

- The change is more modest but this does not show the effect on the spectroscopy of the Lyman and Balmer series.
- Confirms the need for high precision of the underlying atomic data.
- And correctness of the CR model.
Density variation and metastable evolution

*eg*, intermediate-coupled (resolved in J) argon

- Ne = $10^9 - 10^{14}$ cm$^{-3}$.
- Higher lying metastables are sensitive to density.

- Ar$^0$ into a 7.5eV/10$^{14}$ cm$^{-3}$ plasma.
- Ar$^3+$ is the dominant stage in these conditions.

### Table

<table>
<thead>
<tr>
<th>State</th>
<th>Quantum Numbers</th>
<th>Energy (eV)</th>
<th>Abundance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ar$^0$</td>
<td>1 $3s^2 3p^6$</td>
<td>(1)$0(0.0)$</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>2 $3s^2 3p^5 4s^1$</td>
<td>(3)$1(2.0)$</td>
<td>93143.8</td>
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<tr>
<td></td>
<td>3 $3s^2 3p^5 4s^1$</td>
<td>(3)$1(1.0)$</td>
<td>93750.6</td>
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<tr>
<td></td>
<td>4 $3s^2 3p^5 4s^1$</td>
<td>(3)$1(0.0)$</td>
<td>94553.7</td>
</tr>
<tr>
<td>Ar$^+$</td>
<td>1 $3s^2 3p^1$</td>
<td>(2)$1(1.5)$</td>
<td>0.0</td>
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<tr>
<td></td>
<td>2 $3s^2 3p^1$</td>
<td>(2)$1(0.5)$</td>
<td>1431.6</td>
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<tr>
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<td>3 $3s^1 3p^1$</td>
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<tr>
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<td>4 $3s^2 3p^1$</td>
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<tr>
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<td>132481.2</td>
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<td>6 $3s^2 3p^1$</td>
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<td>7 $3s^2 3p^1$</td>
<td>(4)$2(0.5)$</td>
<td>132737.7</td>
</tr>
</tbody>
</table>
Cowan plane wave Born (adas8#1) modified following Mons approach of Quinet et al, J Phys B43 (2010)

Ground state: 3d10 4s2 4p6 4d10 4f14 5s2 5p6 5d1.

Note that 6s is metastable and is lower lying than 5f configuration – a ‘problem’ common to the lowly-ionized tungsten ions.

Thulium-like $W^{5+}$.

$Te(\text{peak}) = \sim 10eV$

$Ip(W^{5+}) = 64.7eV$. 

Tungsten – density effects and metastables
Tungsten – excitation data for the lowly ionized ions

- Ground state: $3d^{10} 4s^2 4p^6 4d^{10} 4f^{14} 5s^2 5p^6$.
- The lowering of 6s is not an issue here and the 1st excited configuration is from the promotion of 4f: $4d^{10} 4f^{13} 5s^2 5p^6 5d^1$
- Photon emissivity coefficients based on Cowan excitation data are compatible with HULLAC calculations (Dong et al, Nuc. Fusion, 59 (2019))
- Ewa Pawelec/Kerry Lawson has observed these lines at JET.
- Contribution function folds abundance and PEC to localize emission layer temperature.
- Lines are not sensitive to a simple confinement time mimic for transport.

- Erbium-like W$^{6+}$.
- $T_e(\text{peak}) = \sim 21\text{eV}$
- $I_p(W^{5+}) = 122\text{eV}$. 
Neutral tungsten

W⁰ can be a measure of influx of tungsten: \( \Gamma = \frac{S}{XB} \times I \)
- Requires ionization (S), excitation (X) and structure atomic data.
- Dominant lines are in VUV which are connected to ground.
- But practical measurements are in visible but are driven by metastables.
- Lower levels are metastable – all with significant population.
- Active area of interest, in particular for ionization data.
ADAS uses ECIP (exchange classical impact parameter) for ionization out of excited levels – empirical formula developed by comparing measured ionization cross sections of light elements. But it is robust and is non-divergent.

This pathway may be larger than the rate from ground.

No convergence to a consensus yet and the spread is too wide to use for an uncertainty analysis.

An outstanding challenge for ab initio calculations and experiment.
Complex lower stages due to 6s and 6p – complicates atomic structure.

Multiple metastables complicates the spectral model.


R-matrix for W\(^+\) – coming (see Connor Ballance’s talk)

R-matrix for W\(^3+\) - C Balance et al., J Phys B46 (2013)

More in the pipeline? DW may be sufficiently good at this point.

CADW for ionization and AUTOSTRUCTURE for DR/RR recombination data but these must be verified by models and experiment.
One outcome of the power optimization work is a set of adf04 excitation data in collision strength (cross sections) and effective collision strength (rates) forms. These can be applied to spectral problems. Mono-energetic ADAS population model, producing a spectral feature, fitted to an EBIT spectrum with ADAS feature-fitting LSQ code. Goal is to apply (shifted) features to tungsten emission from tokamaks.
Tungsten in core

- $4f^n$ DR still an issue
- But now constrained from both sides
- But it’s the pedestal region for JET (100-1000eV)

- Preval et al,
- 73 – 56: PRA 93, 042703 (2016)
- 27 – 14: calculations underway
- 13 – 1: JPB52, 025201 (2109)

Optimised configuration choice for power calculations – year 42
• with increasing Z the peak n for DR reduces (and may be supressed by density) but the peak n for CX moves upwards so CR models will be needed.
• Active CX for mid-Z, ~W^{26+}, are observed transiently at JET.
• Cross section data is not extensive.

• Cross section data for W^+ and W^{2+} exchanging with neutral H/D/T do exist.
• And for W^0 as the donor.
• Not yet included in edge transport models?

ADAS universal fit for CX cross sections

I Yu Tolstikhina (J Phys B45, 2012)
Conclusions and outlook

- A lot of progress has been made in measurements, analysis, calculations and models.
- To answer the tungsten question for tokamaks input from many other areas was, and is, needed – storage rings, EBITs, linear plasmas, table-top experiments, theoretical advances and high performance computing.
- Hydrogen is similar but with a longer history.
- Still some missing pieces – DR, $W^0$ ionization, forbidden lines, spectral features.
- But tungsten emission can now be used as a quantitative diagnostic in fusion.
- Collisional-radiative effective data for modelling is more available.

Validation of atomic data for mid-Z shows convergence.
- Do we need something similar for data used to model and diagnose the edge plasma?

Y Ralchenko (Plas Fus Res B8, 2013)