A consistent set of atomic data for various elements in a fusion reactor
(passive emissions / radiative losses)

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Thanks to: M. O’Mullane, R. Dux, A. Foster
Overview

- Motivation
  - Impurities in Fusion Plasmas
  - Issues with existing data

- New Calculations using ADAS codes
  - What quality has the new data?
  - First tests with the new data

- First Applications of the new data

- Course of Action?
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Impurity Sources
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- Erosion from first wall (e.g. W, Be, C.....)
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- Production of He in reactor core

\[ ^2_1D + ^3_1T \rightarrow ^4_2He + ^1_n \]

3.5MeV 14.1MeV

T. Pütterich, ADAS Workshop 2015, Catania
Impurity Sources

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- Production of He in reactor core

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- Intentionally injected impurities (e.g. N, Ne, Ar, Kr...)

T. Pütterich, ADAS Workshop 2015, Catania
Radiative Losses from Plasma: Need Atomic Data for Many Elements!

Cooling Factors (H. Lux, ADAS WS 2014)

- **Strategy:**
  - Take what is available
  - Various calculation qualities
  - Systematic trends might be hidden
  - Not all data optimized for application in a reactor
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What data was calculated I – What elements?

<table>
<thead>
<tr>
<th>Period</th>
<th>Group</th>
<th>Atomic Number</th>
<th>Symbol</th>
<th>Name</th>
<th>Atomic Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

1Based upon 12C. 1 indicates the mass number of the longest-lived isotope.
What data was calculated I – What elements?

The Periodic Table of the Elements:

**Atomic Properties of the Elements**

### Frequently used fundamental physical constants

For the most accurate values of these and other constants, visit physics.nist.gov/constant.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Speed of light in vacuum</td>
<td>$c = 299,792,458 \text{ m/s}$</td>
</tr>
<tr>
<td>Plank constant</td>
<td>$h = 6,626,756 \times 10^{-34} \text{ J s}$</td>
</tr>
<tr>
<td>Elementary charge</td>
<td>$e = 1.602,177 \times 10^{-19} \text{ C}$</td>
</tr>
<tr>
<td>Electron mass</td>
<td>$m_e = 9.109,389 \times 10^{-31} \text{ kg}$</td>
</tr>
<tr>
<td>Proton mass</td>
<td>$m_p = 1.672,622 \times 10^{-27} \text{ kg}$</td>
</tr>
<tr>
<td>Rydberg constant</td>
<td>$R_n = 10,973,731,569 \text{ m}^{-1}$</td>
</tr>
<tr>
<td>Boltzmann constant</td>
<td>$k = 1.380,649 \times 10^{-23} \text{ J/K}$</td>
</tr>
</tbody>
</table>

### Physical Measurement Laboratory

- [NIST](https://www.nist.gov/)

### Standard Reference Data

- [NIST](https://www.nist.gov/)

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1. Based upon $^{133}Cs$. $^{1}$ indicates the mass number of the longest-lived isotope.
2.*IUPAC* conventional atomic weights; standard atomic weights for these elements are expressed in italics; see IUPAC.org for an explanation and values.
New data has:
Excitation+population model: baseline
Recombination data: baseline
Ionisation data: elevated

But: baseline is not equal to baseline!
New data has:
Excitation+population model: baseline
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But: baseline is not equal to baseline!
New data has:
Excitation+population model: baseline (Cowan + p-w Born + basic CR)
Recombination data: baseline (ADAS407/408 type A, parametric forms)
Ionisation data: elevated (CADW, but in zero-density approx.)

But: baseline is not equal to baseline!
What configurations have been included?

- Try to maximise number of configs
- Include the 'important' configs

**Strategy:**

- Use configurations as identified for W
  (PhD Pütterich, PPCF 2008, NF 2010)
- Level resolved calculations for
  - Predicting spectra
  - Running adas407/408
- Configuration averaged calculations for cooling factors
Configuration Average is Good for Radiated Power

- Level-resolved LR
- Config.-average CA
  - LR set of configs
  - Large set of configs ~#30

Radiated Line Power ($C_{\text{line}}$)

\begin{align*}
\text{Mo-like } W^{32+} & : 4d^6, 4d^54f \rightarrow 4d^55f, \\
& \quad 4p^54d^7, \\
& \quad \sum = 7
\end{align*}

\begin{align*}
\text{LR/CA-LR} & : 4d^6, 4d^54f \rightarrow 4d^55g, \\
& \quad 4p^54d^7 \rightarrow 4p^54d^65g, \\
& \quad 4s4p^64d^7 \rightarrow 4s4p^64d^65g, \\
& \quad 3d^94s^24p^64d^7 \rightarrow 3d^94s^24p^64d^65g; \quad \sum = 28
\end{align*}

Pütterich NF 2010
Ionization Equilibrium for Old Data (Xe)

Ionization Equilibrium of Xenon (Z=54)

This is 3d10

This is 3s1
Ionization Equilibrium for Old Data (Kr)

Ionization Equilibrium of Krypton (Z=36)

This is 3s1

This is 3d10
Ionization Equilibrium of Krypton (Z=36)

This is 3d10

This is 2p6
Ionization Equilibrium for New Data Credible (Kr)

Ionization Equilibrium of Krypton (Z=36)

This is 3d10

This is 2p6

fractional abundance

Te [eV]

0+ 1+ 2+ 3+ 4+ 5+ 6+ 7+ 8+ 9+ 10+ 11+ 12+ 13+ 14+ 15+ 16+ 17+ 18+ 19+ 20+ 21+ 22+ 23+ 24+ 25+ 26+ 27+ 28+ 29+ 30+ 31+ 32+ 33+ 34+ 35+ 36+

4s2 3d10 3p6 3s2 2p6 2s2 1s2
Ionization Equilibrium for New Data Credible(Xe)

This is 3d10
This is 2p6

Ionization Equilibrium of Xenon (Z=54)
Old vs. New Data for H

- Old data up to ~40keV available
- Continuum Radiation in agreement slight deviations for line radiation
- For low-Z, old data may be better for line rad. (or not?)
Old vs. New Data for He

- Old data up to ~40keV available
- Continuum Radiation in agreement slight deviations for line radiation
- For low-Z, old data may be better for line rad. (or not?)
- Helium: Continuum rad. In old data has wrong T-dependence - extrapolation?
Old vs. New Data for H to Ne

- Old data up to ~40keV available
- Continuum Radiation in agreement slight deviations for line radiation
- For low-Z, old data may be better for line rad. (or not?)
- Helium: Continuum rad. In old data has wrong T-dependence - extrapolation?
New Data Behaves Straight Forward
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How Much of an Impurity is Tolerable in a Fusion Reactor?

- All reactor models require cooling factors to model impurity radiation.
- Here, very simple 0.5D model is used to evaluate impurity limit for each element.

\[ \rho^* = \frac{\tau_{He}}{\tau_E} \]

- 0D Model \( \rho^* = 5 \)
- T-peaking (2.5) \( \rho^* = 5 \)
- T- & n-peaking (2.5 & 2.5) \( \rho^* = 5 \)
- Match DEMO1 (2.0 & 1.3) \( \rho^* = 5 \)
- Match DEMO1 (2.0 & 1.3) \( \rho^* = 1 \)
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Summary – Outlook

- Data for plasma emissions have been calculated for all ions of 35 elements

- The same procedure has been used for all elements, thus systematical trends in the data can be better observed

- The quality is good for baseline calculations

- For elements with Z higher than ~18 the new data is probably an improvement

- Include all data in ADAS? Dedicated benchmarking?