Ionisation cross sections and ionisation balance

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Overview

- Methods of generating ionisation cross sections.
- New ionisation data for ADAS.
- Recent findings:
  - Importance of the near threshold region
  - Experimental measurements of metastable fraction.
- Ionisation project results.
- Future work.

Method of generating ionisation cross sections

- Experimental measurements
  - Most experiments don't know the metastable fraction.
- Theory
  - *Semi-empirical and classical* (e.g. Lotz, ECIP)
  - *Perturbation theory*
    - Distorted-wave [Not good for near neutrals or excited states]
  - *Non-perturbative methods*
    - R-matrix with pseudostates (RMPS)
    - Time-dependent close-coupling (TDCC)
    - Converged close coupling (CCC)
    - Exterior complex scaling (ECS)

New data in the last year

- Iso-nuclear work (Configuration-average distorted-wave: CADW)
  - Xe
  - Sn
  - Ar[1]
- Non-perturbative calculations
  - Neutral Ar [RMPS][2]
  - Be-like C, N and O [RMPS]
  - Li^+ 1s2s (^3S) [TDCC & RMPS][3]
  - B [TDCC & RMPS][4]
- Isoelectronic sequences
  - H-like
  - He-like
  - Li-like

[1]*Loch et al. Phys. Rev. A* ***76*** *022706 (2007)*
[2]*Ballance et al. J. Phys. B* ***40*** *F27 (2007)*
[3]*Berengut et al. J. Phys. B* ***40*** *1331 (2007)*
[4]*Ballance et al. J. Phys B* ***40*** *1131 (2007)*

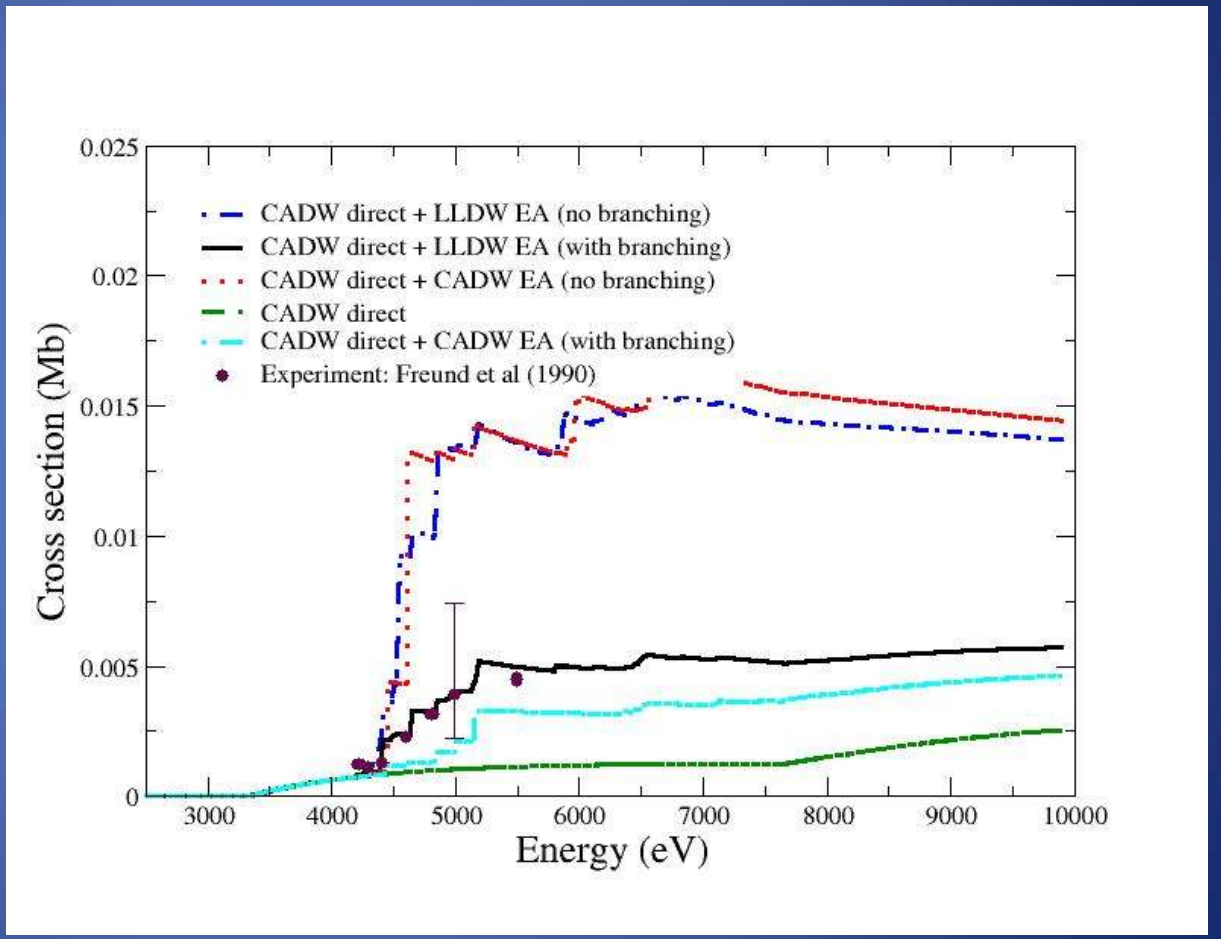
Processing the adf23 files

- The new data is produced in adf23 format.
- Various utility codes can process the files. These will:
  - Make S-lines that can be added to an adf04 file.
  - Make a zero-density scd adf11 file from a set of adf23 files for an element.
- We also have some tools for more automatic checking of the new data against existing ADAS data.

Iso-nuclear calculations

Example: Xe^{43+}

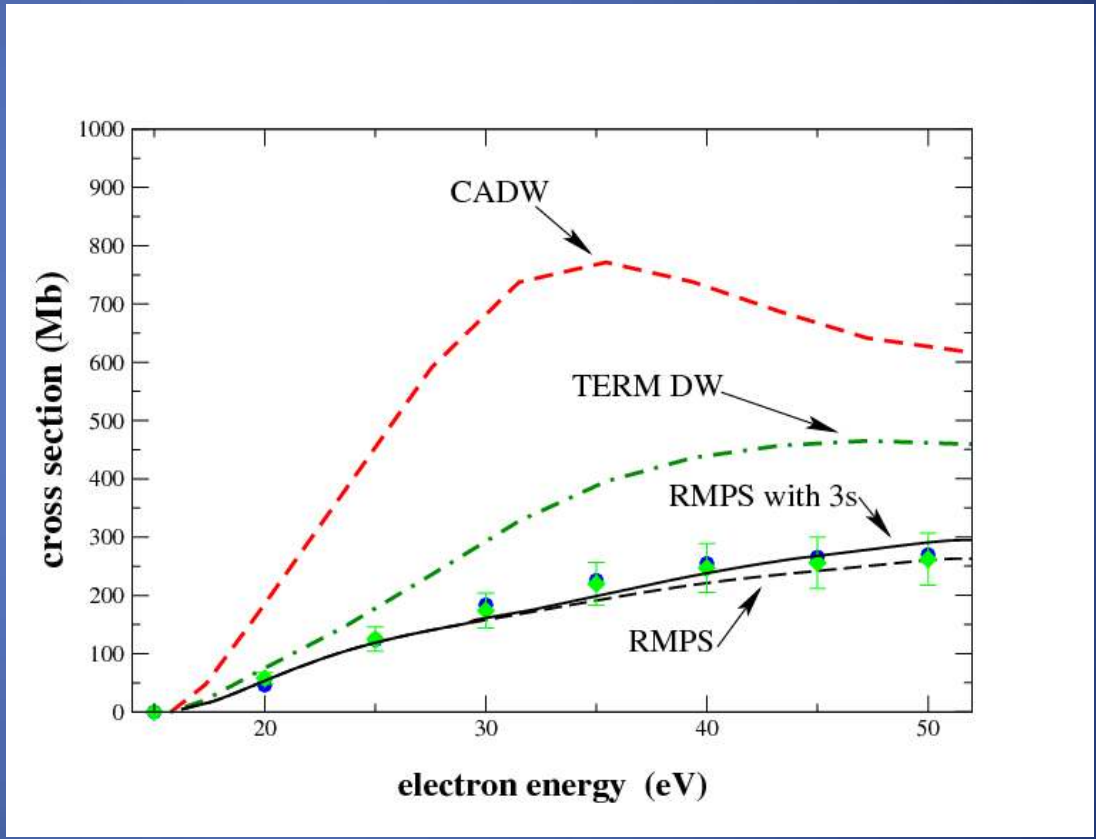
- For our iso-nuclear work we use the CADW method to calculate
  - Direct ionization
  - Excitation-autoionisation
- This method generally does very well, except for near neutrals.
- For certain ion stages the excitation-autoionisation contribution can be very large.
  - Radiative decay damps the excitation-autoionisation for the higher ion stages.



Iso-nuclear calculations

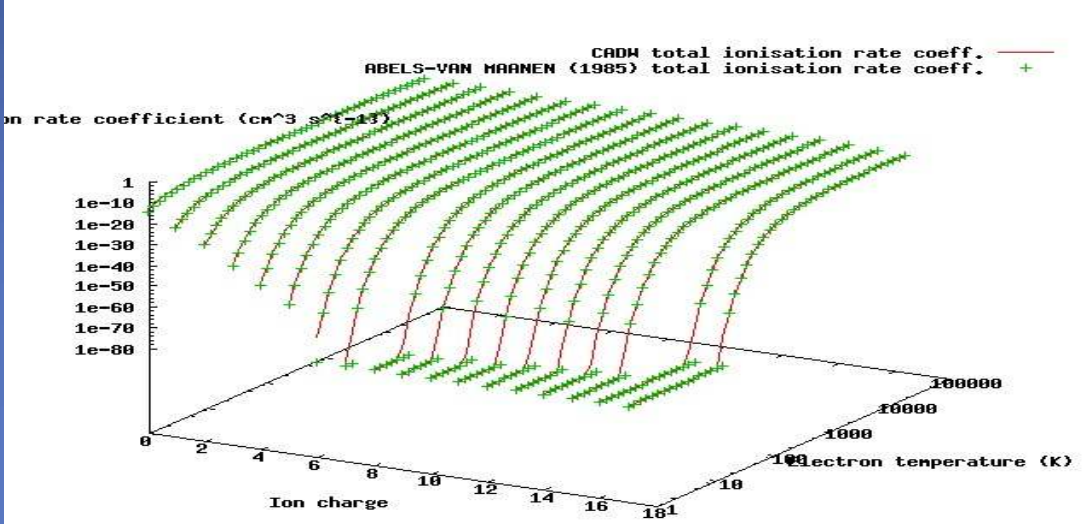
Example : Neutral Ar

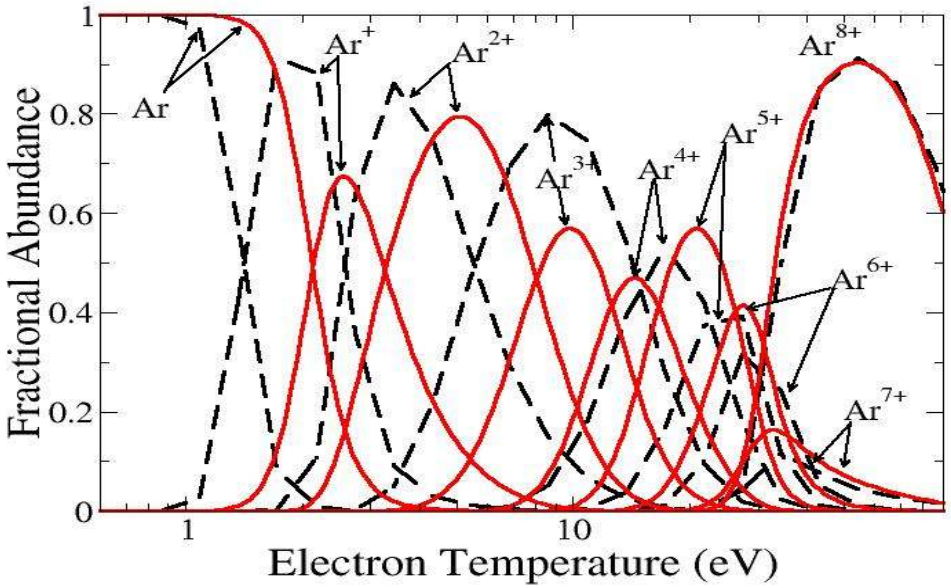
- The DW methods usually overestimate the near neutral ionisation cross sections.
- Thus, non-perturbative methods generally have to be used for the near neutrals.
  - The RMPS method was used to calculate the ionisation cross section of neutral Ar.
  - Good agreement with experiment was found.



Ar ionisation balance

- We calculated the low density ionisation balance of Ar using the new data.
  - We also included new CADW dielectronic recombination for the low ion stages.
  - The new data makes a difference to the abundances of the near neutral ion stage.
- The predicted abundances appear to be verified with a plasma experiment at Auburn University.



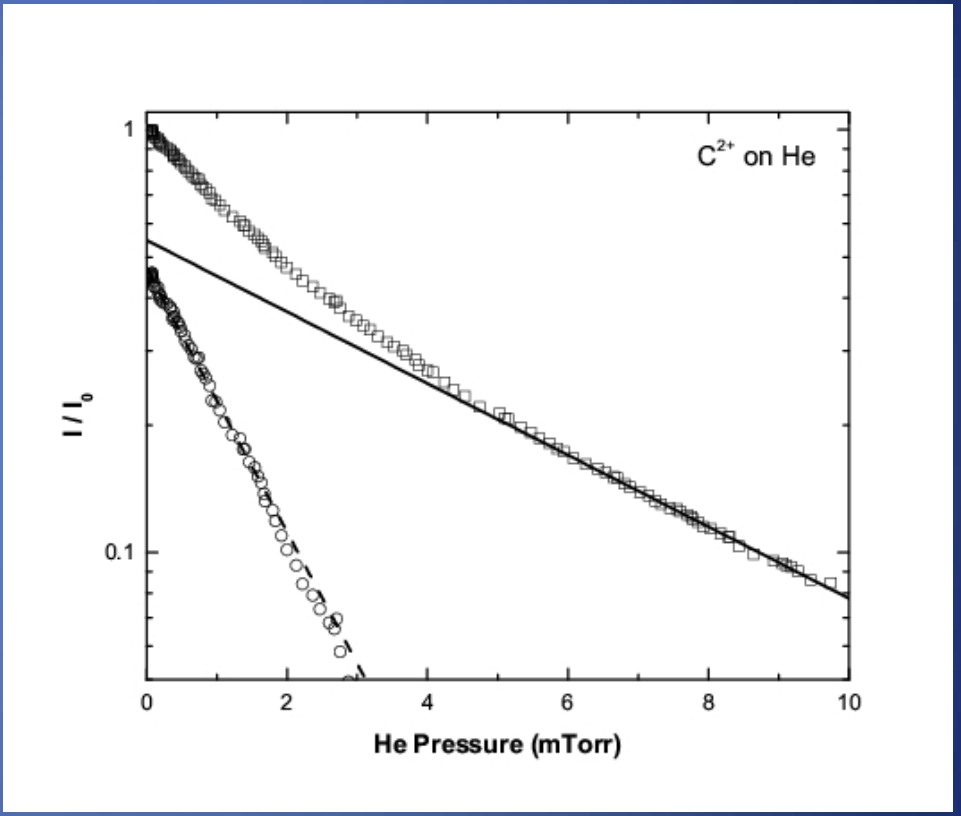


New experimental measurements

Be-like ions

- An experimental technique recently implemented at the Oak Ridge National Laboratory allows the metastable fraction to be measured in ionisation cross section experiment.
- Measurements were made on
  - C^{2+} (46 ± 7)%
  - N^{3+} (30 ± 6)%
  - O^{4+} (24 ± 7)%
- The results were compared with RMPS and CADW theory data.

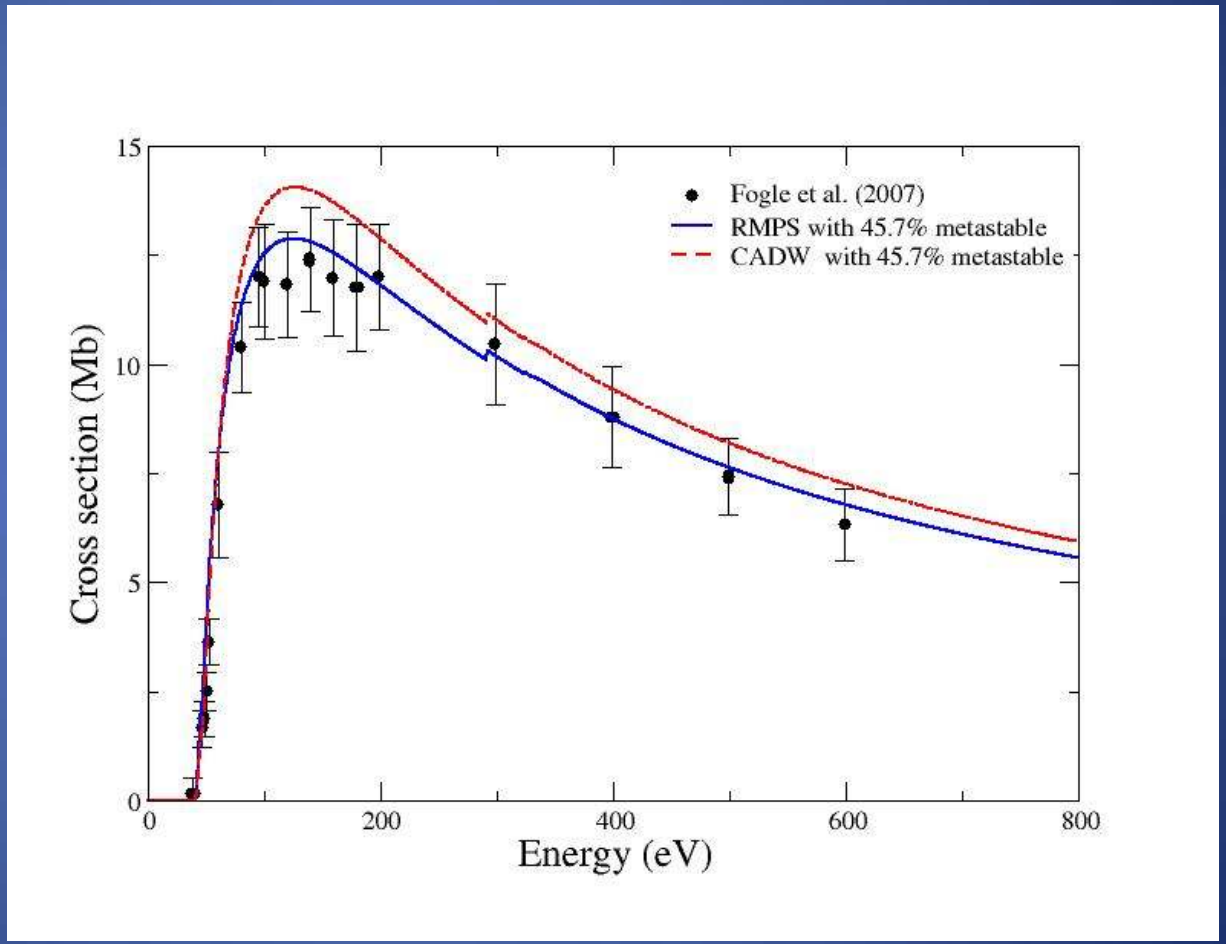
Fogle et al. The Astrophysical Journal (in press)



Gas attenuation measurements for C^{2+}

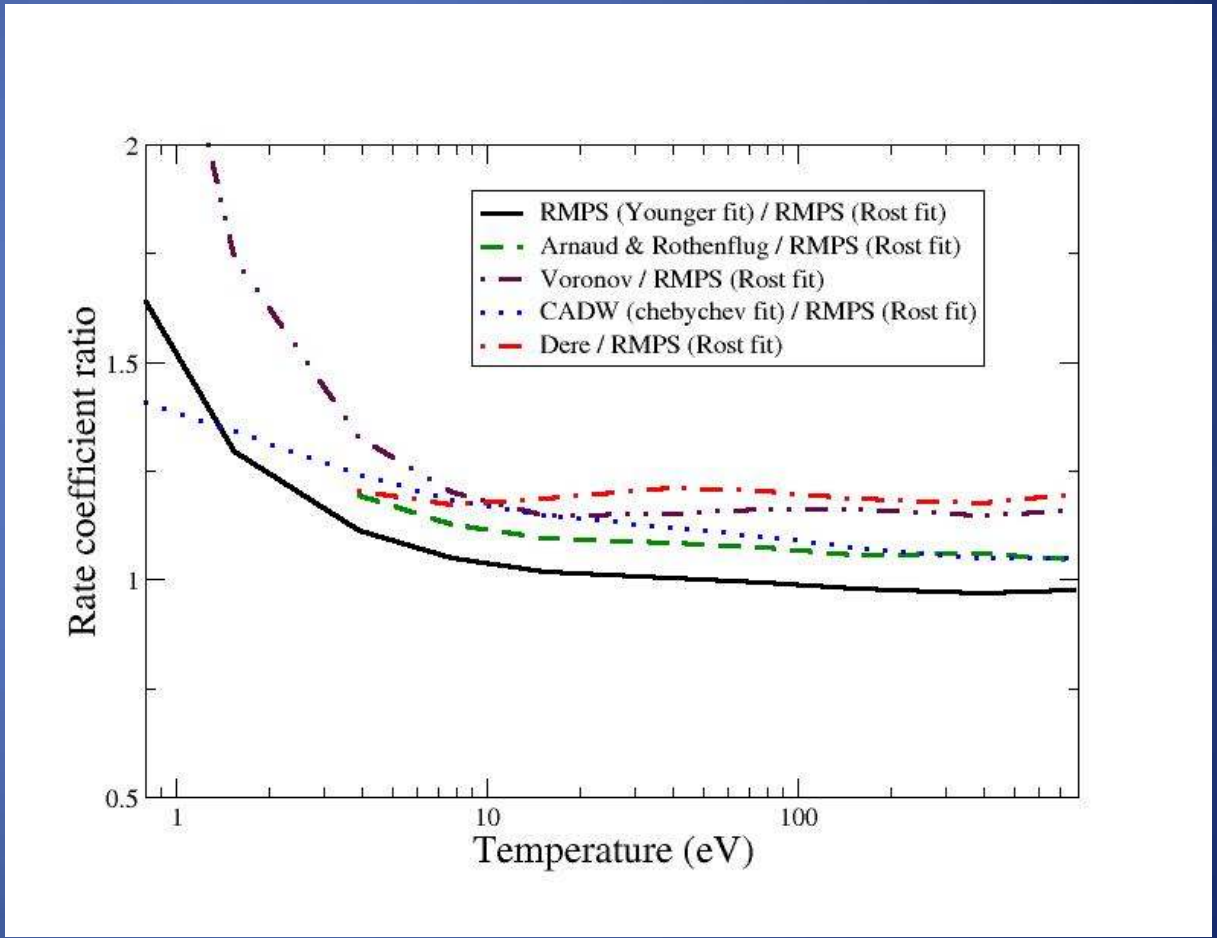
ORNL C^{2+} cross section comparison

- The RMPS results are in good agreement with experiment
- The CADW results lie above the measured cross section.



C^{2+} rate coefficients

- The ions start to have significant abundance at ~0.1 of the ionisation potential.
- The low temperature rate coefficients sample mostly the near threshold part of the cross section.
  - The rate coefficients are very sensitive to the fitting of this region.
  - A Rost fit, or a Chebychev polynomial fit is recommended.



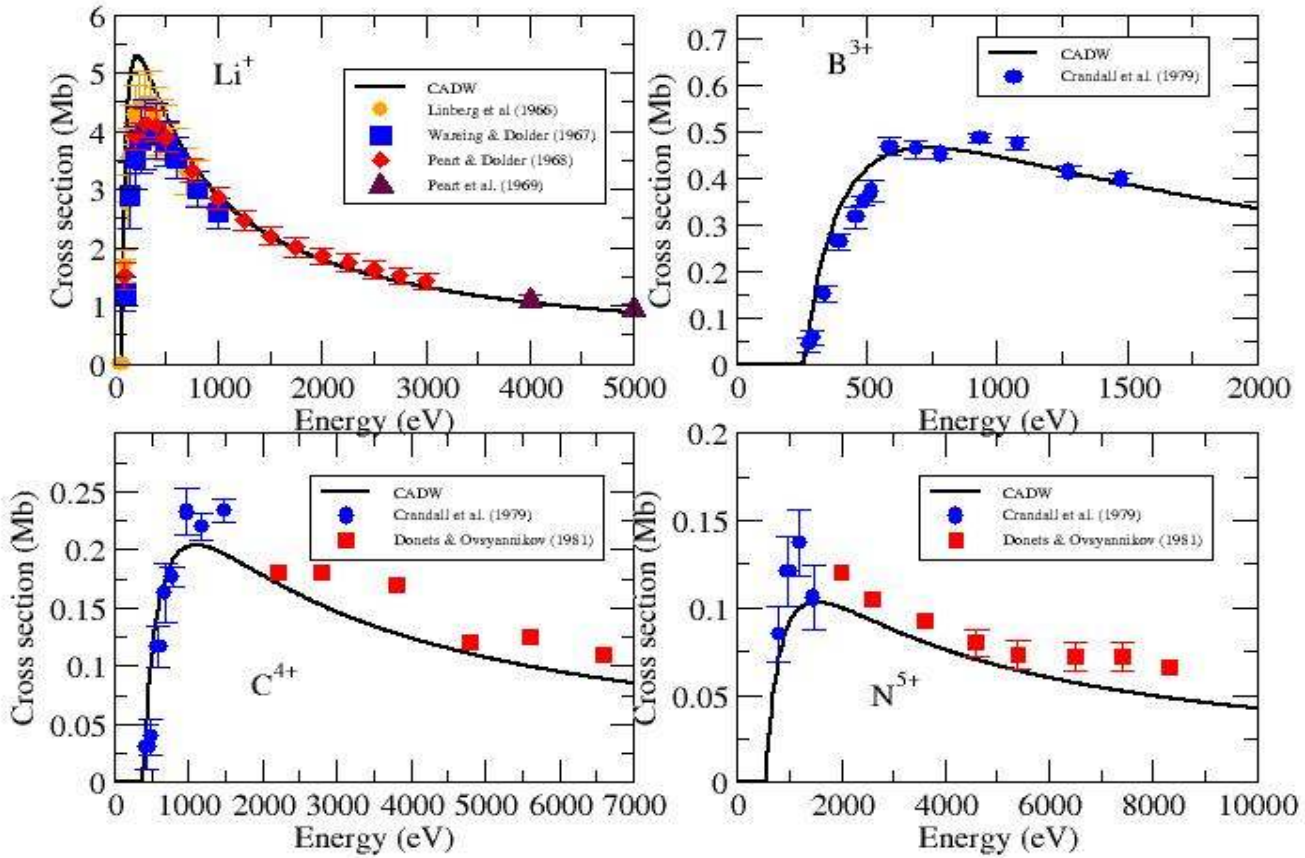
The ionisation project

- An ADAS project aimed at the large scale generation of ionisation rate coefficients is now producing data.
- The data consists of
  - CADW direct ionization, that is then level-resolved via some angular factors.
  - CADW excitation to autoionising configurations.
  - Level-resolved Auger yields (from Autostructure)
- The data is metastable resolved for both initial and final ion stages.
- The idea is to work through iso-electronic sequences in a similar way to the `DR project'.

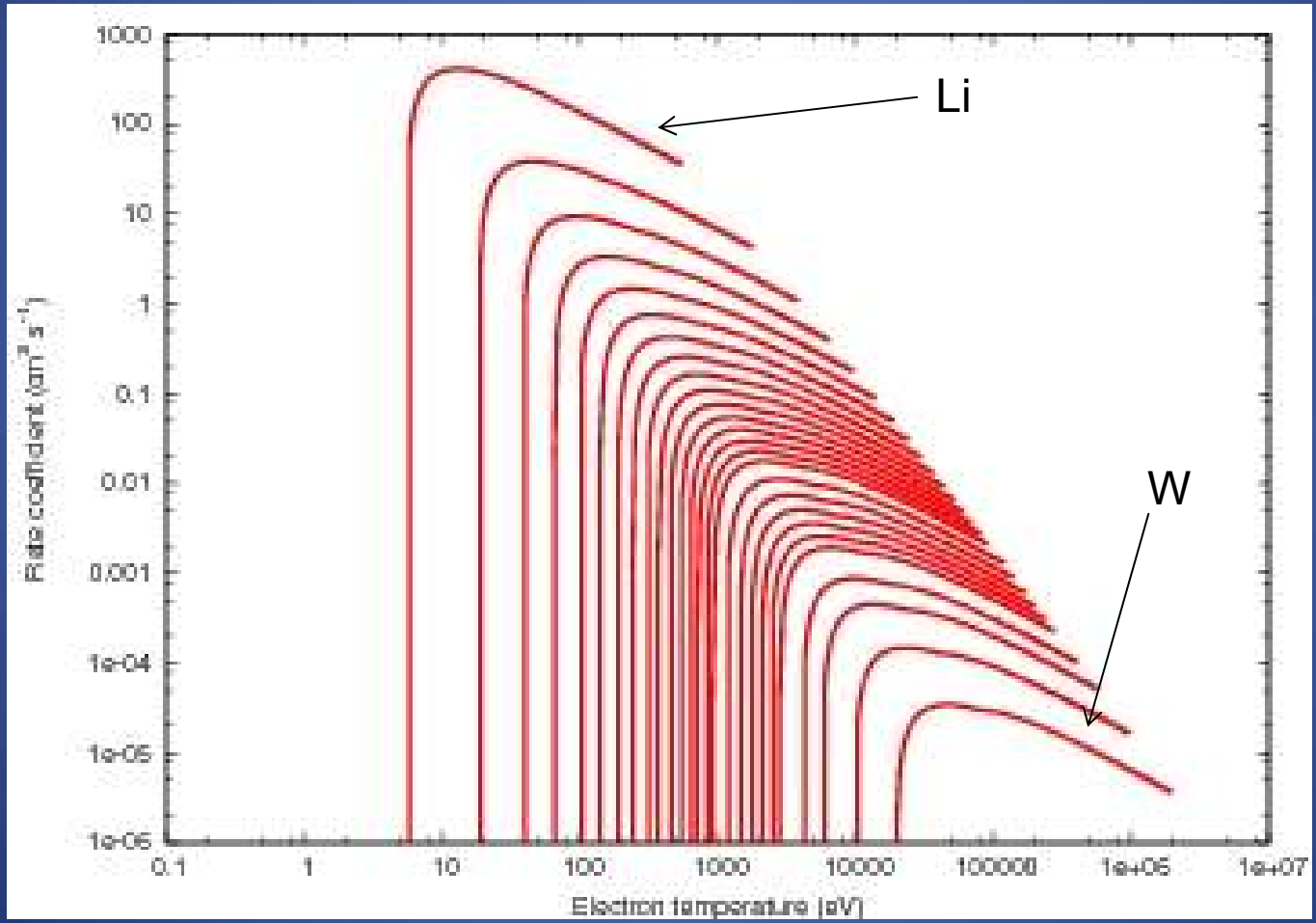
Recent results

- Data is completed for the
  - The H-like isoelectronic sequence
    - 1s, 2s
  - The He-like isoelectronic sequence
    - $1s^2$, 1s2s (^3S & ^1S)
  - The Li-like isoelectronic sequence.
    - $1s^22s$
- Calculations are underway for the Be and B-like sequences.
- The plans are to continue along the iso-electronic sequences.
- The near neutral ion stages often already have non-perturbative calculations for them. If this is the case, the non-perturbative data is used.

Selected He-like cross sections



Iso-electronic rate coefficients Li-like ions



Future plans

- We will continue working through the iso-electronic sequences for the ionisation project.
- The main challenge remaining for ionisation is the near neutral heavier species (and a few of the lighter ions).
  - Thus we intend to use the RMPS and TDCC methods to improve the data available for these systems.
  - Let us know if there are particular ion stages you would like us to set up.
- We also intend to look into improving the ionisation data for excited states.