Assembling atomic data for diagnosing and modelling fusion plasmas

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Spectroscopy of plasmas

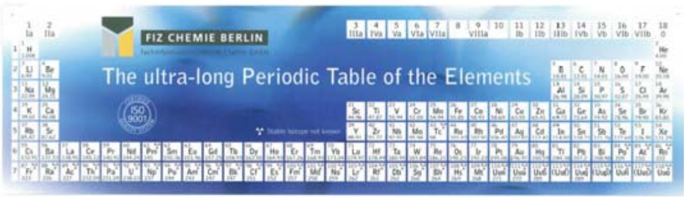
If we wish to interpret the emission from plasmas:

- Require atomic and molecular data
- Not necessarily of highest quality – completeness is as important
- What do we mean by atomic data?
- Fundamental data mediated via models to be useful for modelling and diagnostic use.
- Like a parameterization of atomic features with macroscopic plasma quantities (Te, Ti, Ne, B, I etc.).
- Large amounts of data involved.

Necessary tasks:

- Gather/calculate fundamental data.
- Develop appropriate (collisional-radiative) models.
- Store data in a well defined way.
- Assess the quality of the data.

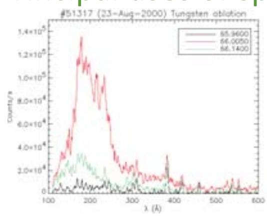
Scope of the challenge



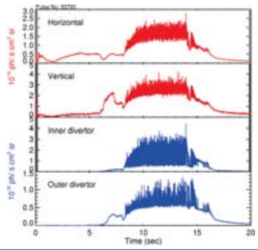
Set some limits:

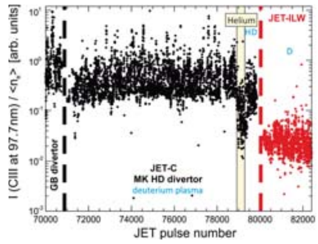
- Consider elements and models appropriate for magnetic confined fusion – and related plasma such as solar .
- Model collisional, non-LTE, (mostly) optically thin plasmas.
- Limit number of elements.

Principal uses of spectroscopic measurements



- Information on state of plasma.
- Control of plasma performance.
- Assessment of machine and scenarios state.
- Not a light source.





ADAS is one approach – what is it?

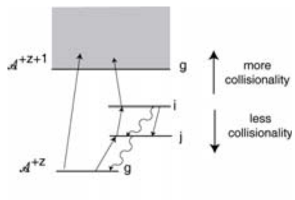
- ADAS, as a database delivers:
  - extensive set of fundamental and derived data tuned for plasma modelling and spectroscopic analysis,
  - provides 'baseline' level data for any element and ion stage.
  - atomic data source for many modelling codes and systems,
  - makes a significant quantity of data publically available via OPEN-ADAS http://open.adas.ac.uk (with IAEA).
- ADAS, as a computer system, is designed to:
  - provide a set of interactive codes which are easy to use,
  - provide subroutine libraries for inclusion in other codes,
  - allow direct access to diagnostically relevant data.
- ADAS, as a collaborative organisation:
  - provides guidance (training courses, visits etc.) on running codes,
  - gives recommendation on the best data to use,
  - assists in analysis and development of analysis tools and models.

It is structured as a self-funded consortium between most major fusion laboratories and universities. Its historical roots are in JET and is now managed by the University of Strathclyde and is governed by a steering committee of the participating members.

Finite density environment

collisonal-radiative picture for ionisation and recombination

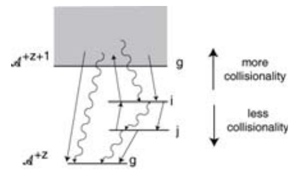
Reactions:



At higher densities, collisional excitation and de-excitation between excited levels compete with spontaneous emission.

$$A^{+z}(i) + e \rightleftharpoons A^{+z}(j) + e$$

Indirect pathways lead to line emission and ionisation may occur in a stepwise manner.



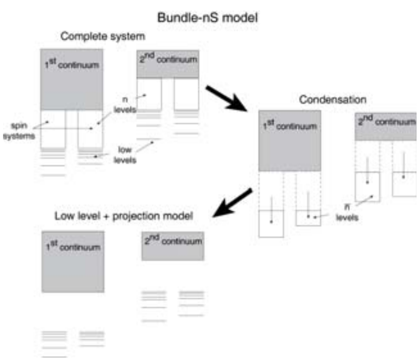
Three-body recombination must be added to the reactions which pairs with collisional ionisation from excited states

$$A^{+z}(i) + e \rightleftharpoons A^{+z+1}(g) + e + e$$

Not all recombinations lead to growth of the ground population of the recombined ion.

Finite density environment

generalized collisonal-radiative approach – projection of high-n levels

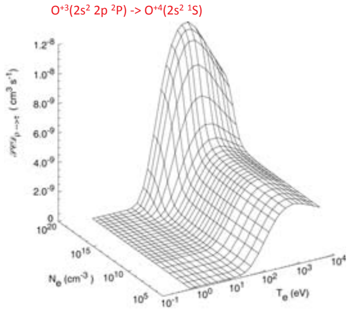


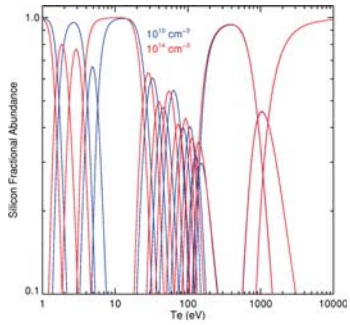
- For light/medium weight elements there is a truncation problem since the true atom with its infinite number of Rydberg states.
- Dielectronic recombination populates high lying states.
- Setup a bundle-n collisional-radiative matrix for the whole system. Use the inverse sub-matrix propagator for the ry n-shells to project onto the ry_{ls} n-shells.
- Eliminate the direct couplings and expand statistically over the ry_{ls} nS-shell substructure and add to the more exact collisional-radiative matrix for ry.

Coefficients are functions of T_e *and* N_e

The **SCD** coefficient increase to a new limit at high density as excitations lead to ionisation

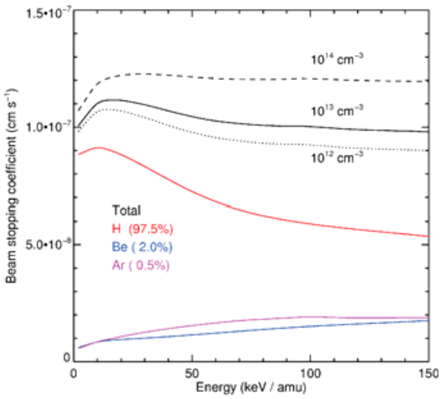
$O^{+3}(2s^2\ 2p\ ^2P) \rightarrow O^{+4}(2s^2\ ^1S)$





With Silicon the effect is greater effect at edge than in core

Beam stopping coefficients are also dependent on the plasma environment



Variation of stopping due to density effects is similar to the influence of impurities as stopping species.

The 3 types of data files in ADAS

- **Derived data** are data tailored for modelling: electron temperature and density dependent effective emission coefficients, effective ionisation/recombination rates, radiated power, spectral emissivities, beam stopping, spectral features etc.,
  - Result of fundamental data processed via population models.
  - Much of this data are **not** catalogued in traditional data centres.
- **Fundamental data** are core atomic data necessary for modelling: A-values, energy levels, cross sections, collision strengths, zero density ionisation rates etc.,
  - Many sources: collaborators, literature, self-generated, data centres etc.
  - Many resolutions: from simplistic to the forefront of computational physics.
- **Driver data** allow complete regeneration of all ADAS derived data (and some fundamental data) in conjunction with the various ADAS codes,
  - Unique to ADAS system.

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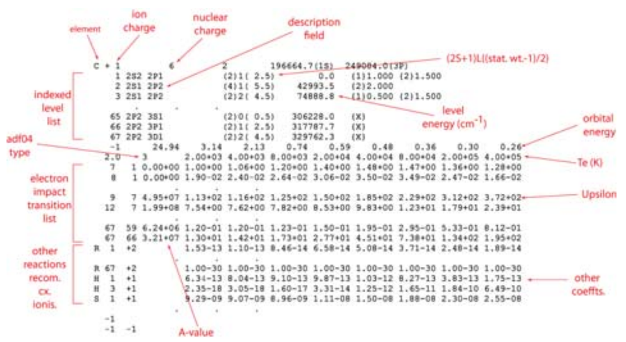
ADAS data formats (*adf*)

All ADAS data is stored in a well defined, tightly specified format – eg. adf 04 file.



A free-format comment section at the end detailing source and responsible person.

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ADAS data and computational overview

There are 55 different ADAS data formats

Some key ADFs and MDFs for general application

ADF01 : charge exchange cross sections
ADF04 : specific ion data
ADF11 : coll.-rad. ionis., recom. and related coefficients.
ADF13 : ionisation per photon ratios
ADF15 : emissivity coefficients
ADF40 : envelope feature photon emiss. coefficients
ADF21 : beam stopping coefficients
ADF39 : photoionization cross sections

MDF00: fundamental diatomic molecular constants
MDF01: rovibronic models
MDF02: fundamental cross-section data
MDF04: specific molecule data

Interactive user interface
ADAS series (9 series with 85 programs)

The application interface
ADAS Fortran subroutine (~1900) , IDL procedure (~1700) and python (~20) routine libraries
Data extraction procedures and subroutines by format: xxdata_<nn> , read_adf<nn>, xxdatm_<nn> , read_mdf<nn> .

Offline-ADAS for large scale production
6 large scale production packages: adas7#1, adas7#3, adas8#1, adas8#2, adas8#3, adas8#4 .

Documentation – manual and course material.

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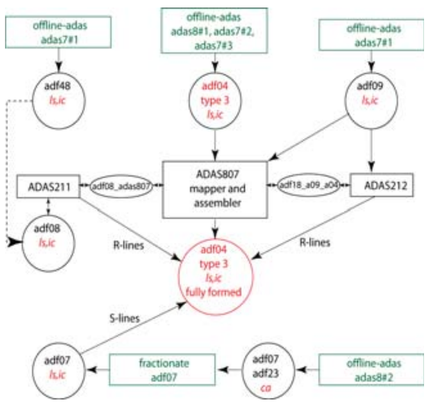
Assembling a high precision adf04 dataset

The schematic shows the inter-connected production codes and pathways which are used to form *adf04* datasets for light and medium weight ions of elements at the highest precision.

- Codes in black letter capitals are part of interactive ADAS.
- The ADAS codes containing '#' are non-interactive offline-adas codes executed in distributed processing by scripts.



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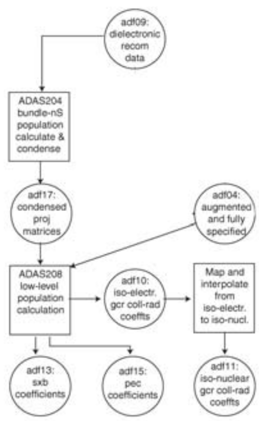
Workflow to generate derived data from fundamental collection



- Data files (*adf*) – fundamental, derived and driver – are tightly defined and have ADAS supplied reading routines.
- ADAS codes operate on *adf* datasets and output to other *adf* datasets
- Plasma and model options via script or input screen stored in output *adf*.

- Data assembly and processing is too manual a process.
- Origin of the data is held in free-form in the comments section of each file.

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Lithium – only 3 electrons

ELSEVIER

Available online at www.sciencedirect.com
ScienceDirect
Atomic Data and Nuclear Data Tables 92 (2006) 813–851

Atomic Data and Nuclear Data Tables
www.elsevier.com/locate/adt

Generalised collisional-radiative model for light elements.
A: Data for the Li isonuclear sequence

S.D. Loch [a,*], J. Colgan [a], M.C. Witthoeft [a], M.S. Pindzola [a], C.P. Ballance [b], D.M. Mitnik [b], D.C. Griffin [b], M.G. O'Mullane [c], N.R. Badnell [c], H.P. Summers [c]

[a] Department of Physics, Auburn University, Auburn, AL 36849, USA
[b] Department of Physics, Rollins College, Winter Park, FL 32789, USA
[c] Department of Physics, University of Strathclyde, Glasgow G4ONG, UK

- 64 adf datasets
- 43 in OPEN-ADAS: fundamental data (excitation, DR, RR and ionisation)
  derived data (source, power, S/XB and PEC coefficients)

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Lithium – the 64 datasets

Driver for adas8#1 adf04
adf34/lithium/li0.dat
adf34/lithium/li1.dat
adf34/lithium/li2.dat

Baseline adf04 to give baseline fill-in and A-values
adf04/copmm#3/ls#li0.dat
adf04/copmm#3/ls#li1.dat
adf04/copmm#3/ls#li2.dat

R-matrix data from Connor Ballance and Don Griffin
adf04/lilike/lilike_cpb02#li0.dat
adf04/helike/helike_cpb02#li1.dat
adf04/hlike/hlike_cpb02#li2.dat

Metastable and excited state resolved ionisation data from S Loch
adf07/szd02#li/szd02#li_li0.dat
adf07/szd02#li/szd02#li_li1.dat
adf07/szd02#li/szd02#li_li2.dat

State resolved radiative recombination from Nigel Badnell
adf48/nrb05#he/nrb05#he_li1ls.dat
adf48/nrb05#h/nrb05#h_li2ls.dat
adf48/nrb05##/nrb05##_li3ls.dat

State resolved dielectronic recombination from N Badnell and M Bautista
adf09/nrb00#h/nrb00#h_li2ls12.dat
adf09/nrbmb00#he/mb00#he_li1ls12.dat
adf09/nrbmb00#he/mb00#he_li1ls23.dat

Fully specified adf04 file for processing
adf04/adas#3/cpb02_ls#li0.dat
adf04/adas#3/cpb02_ls#li1.dat
adf04/adas#3/cpb02_n#li2.dat

Mapping high-n to low levels
adf18/a17_p208/exp96#li/exp96#li_li0ls.dat
adf18/a17_p208/exp96#he/exp96#he_li1ls.dat
adf18/a17_p208/exp96#h/exp96#h_li2n.dat

Projection matrices
adf17/cbnm96#li/cbnm96#li_li0ls.dat
adf17/cbnm96#he/cbnm96#he_li1ls.dat
adf17/cbnm96#h/cbnm96#h_li2ls.dat

iso-electronic GCR data
adf10/acd96/pj#acd96_li11.dat
adf10/acd96/pj#acd96_li21.dat
adf10/scd96/pj#scd96_li11.dat
adf10/scd96/pj#scd96_li21.dat
adf10/xcd96/pj#xcd96_li12.dat
adf10/xcd96/pj#xcd96_li21.dat
adf10/plt96/pj#plt96_li##.dat
adf10/prb96/pj#prb96_li10.dat
adf10/prb96/pj#prb96_li20.dat

iso-nuclear source and power - resolved
adf11/acd96r/acd96r_li.dat
adf11/scd96r/scd96r_li.dat
adf11/qcd96r/qcd96r_li.dat
adf11/xcd96r/xcd96r_li.dat
adf11/plt96r/plt96r_li.dat
adf11/prb96r/prb96r_li.dat

iso-nuclear source and power - unresolved
adf11/acd96/acd96_li.dat
adf11/scd96/scd96_li.dat
adf11/ecd96/ecd96_li.dat
adf11/ycd96/ycd96_li.dat
adf11/zcd96/zcd96_li.dat
adf11/plt96/plt96_li.dat
adf11/prb96/prb96_li.dat

Ionisations per photon
adf13/sxb96#li/sxb96#li_pjr#li0.dat
adf13/sxb96#li/sxb96#li_pju#li0.dat
adf13/sxb96#li/sxb96#li_pjr#li1.dat
adf13/sxb96#li/sxb96#li_pju#li1.dat
adf13/sxb96#li/sxb96#li_pjr#li2.dat
adf13/sxb96#li/sxb96#li_pju#li2.dat

Photon emissivity coefficients
adf15/pec96#li/pec96#li_pjr#li0.dat
adf15/pec96#li/pec96#li_pju#li0.dat
adf15/pec96#li/pec96#li_pjr#li1.dat
adf15/pec96#li/pec96#li_pju#li1.dat
adf15/pec96#li/pec96#li_pjr#li2.dat
adf15/pec96#li/pec96#li_pju#li2.dat

In OPEN-ADAS

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Most data within ADAS is *ab initio*

GRIFFIN, MITNIK, COLGAN, AND PINDZOLA — PHYSICAL REVIEW A **64** 032718

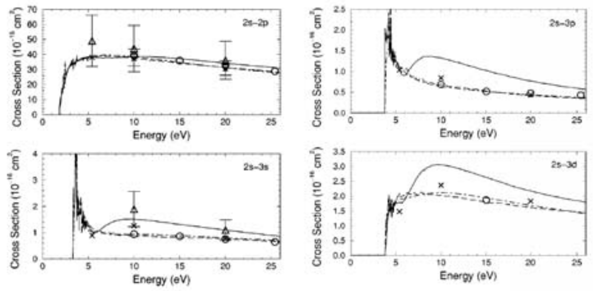


FIG. 2. Total electron-impact excitation cross sections for the $2s \rightarrow 2p$ and $2s \rightarrow 3s$ transitions in Li. Solid curves, present 14-state *R*-matrix calculation; dashed curves, present 55-state RMPS calculation; open circles, present TDCC calculation; dot-dashed curves, from fits to the CCC calculations given by Schweinzer *et al.* [10]; crosses, CCO calculation of Bray *et al.* [9]; upward triangles, experimental measurements of Williams *et al.* [11]; downward triangles, experimental results of Vušković *et al.* [12].

FIG. 3. Total electron-impact excitation cross sections for the $2s \rightarrow 3p$ and $2s \rightarrow 3d$ transitions in Li. Solid curves, present 14-state *R*-matrix calculation; dashed curves, present 55-state RMPS calculation; open circles, present TDCC calculation; dot-dashed curves, from fits to the CCC calculations given by Schweinzer *et al.* [10]; crosses, CCO calculation of Bray *et al.* [9].

Li^0 excitation cross sections

The collisional-radiative model can occasionally be verified by experiment

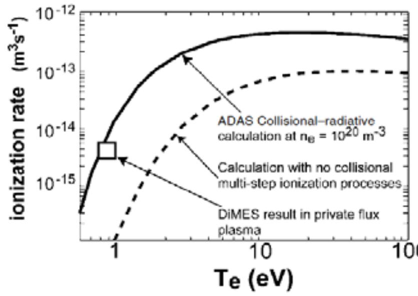


Figure 8. Ionization rate of sputtered lithium atoms as a function of electron temperature under PF plasma bombardment in H-mode plasma. Figure shows how the ADAS collisional–radiative model must be used to explain experimental data from Li–DiMES in PF plasma.

J P Allain *et al*, Nuclear Fusion, **44** (2004) p655

ADAS data and fusion modelling

ADAS data provides data (mostly in derived form) to

- EUROfusion WP-CD (Europe's Integrated Tokamak Modelling workflow)
- Basis of ITER's Integrated Modelling and Analysis Suite (IMAS)
- JET: edge2d, JAMS and sanco
- PPPL: TRANSP via NUBEAM for beam stopping and emission
- CEA: CHRONOS
- GA: UEDGE
- IPP: solps (will be also part of EUROfusion effort)
- CCFE: PROCESS for DEMO design
- ITER: solps and diagnostic design studies
- OPEN-ADAS data used elsewhere but not tracked.

OPEN-ADAS at http://open.adas.ac.uk

Integrated Modelling & Analysis Suite (IMAS)

- Physics modelling tools to support Plasma Operations
  - Validation of pulses prior to operation
  - During shots for plasma control (forecasting) and live display
  - Post-pulse for comprehensive reconstruction using full set of diagnostic measurements
  - Components describing macroscopic behaviour should improve as ITER explores new physics domain of burning plasmas
- Tools must be computationally efficient, robust, well-documented and interface with other systems
  - Must be validated and have associated regressions tests
- Managed by IO and accessible to all ITER Members
  - Use distributed revision control system (git) to promote collaborative development

Simon Pinches, ITER IO

Atomic, Molecular, Nuclear & Surface Data in IMAS

- Systematic recording of atomic data used in IMAS simulations in IMAS database
  - No hard-coded atomic data in codes, no untraceable direct access to external database for atomic data
  - Provenance traceability (recording source of atomic data tables)
- AMNS package provides methods to:
  - Import atomic data tables from other databases (e.g. ADAS) into a local storage (includes recording data provenance)
  - Read atomic data tables from that storage and calculate the requested information (e.g. interpolation of tabular data)

Simon Pinches, ITER IO

Using A/M/PMI data

- ADAS data will be part of larger integrated systems
- Accessing data will probably not be via reading the *adf* ASCII formatted files.

- WPCD uses a CPO – consistent physical object – to store atomic, molecular, surface and nuclear data.
- IMAS calls these IDS – interface data structures.

- CPO/IDS will:
  - Contain just one, recommended, version of a process
  - Will be updated regularly
  - Have a version identifier
  - Permit calling codes to track AMNS version
  - Allow codes to use earlier versions but the default is to used the latest version

- CPO/IDS are not:
  - The canonical version of the data

Avoiding fracturing the data

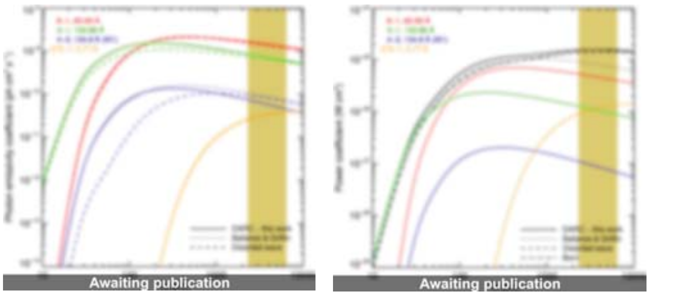
- It has taken a significant amount of time and effort to assemble the ADAS database
- The focus remains on the needs of magnetic confined fusion.
- Data is not added unless there is a clear use
  - Some iso-electronic fundamental data is archived since trend analysis is a powerful technique.
- ADAS is a database with historical data, multiple calculations of the same process and different levels of sophistication co-exist.
- The combination of tightly defined formats, numerical data storage and asymptotically correct extrapolation and splining reading routines has stood the test of time.

- Analysis and modelling are becoming larger-scale enterprises and different ways of accessing the data, tracking its provenance and propagating model re-runs based on updated recommended data will be necessary and expected.
- ADAS remains the canonical source – the AMNS CPO/IDS will extract a 'best data' recommendation for practical use.
- AMNS CPOs are written by ADAS personnel – currently with a program which extracts ADAS data with ADAS routines which then writes the CPO over a large grid of plasma parameters.

Reliability and quality of atomic data

- Data provenance – where does it come from.
- Data quality – how good, or how close to reality, is it.
- Completeness – is the physics description complete?

Consider W^{44+} ($3d^{10}\,4s^2$) a new calculation, yielding a range of values and showing the effect of omitting a configuration ($3d^9\,4s^2\,4f$).



W^{18+} dielectronic recombination

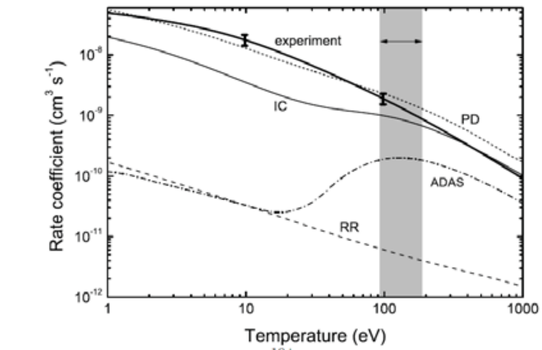
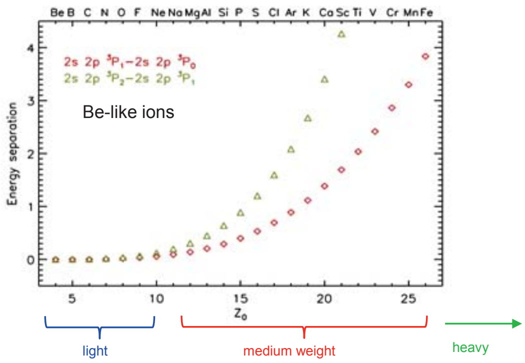


Fig 4. Plasma recombination rate coefficients for W^{18+} (Spruck et al. Phys.Rev.A At Press, 2014). Thick solid curve: experimentally derived rate coefficient; thin solid curve: IC theory; short-dashed curve (PD) partitioned and damped calculation; Dot-dashed curve: ADAS plasma recombination rate coefficient (Foster 2008).

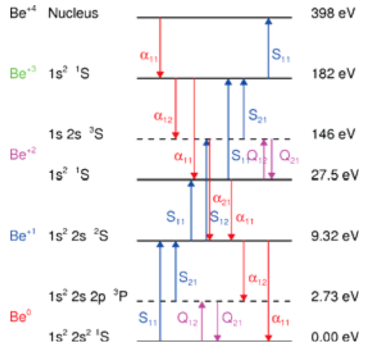
Intermediate coupling and fine structure



Cannot ignore the divergence for Z>10

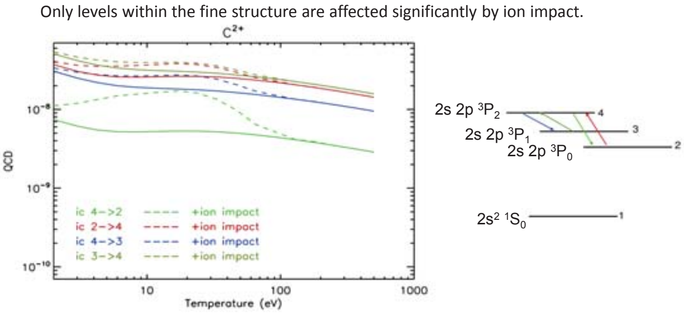
GCR coefficients

$$\frac{dN_\rho^{+z}}{dt} = -(N_e S_{CD,\sigma\rightarrow\nu} N_\sigma^{+z} + N_e \alpha_{CD,\nu'\rightarrow\rho} N_{\nu'}^{+z+1} + N_e Q_{CD,\sigma\rightarrow\rho} N_\sigma^{+z}) + \ldots$$



Q_{CD} – metastable cross-coupling

Only levels within the fine structure are affected significantly by ion impact.



$$Q_{CD,\sigma\rightarrow\rho}^{total} \simeq Q_{CD,\sigma\rightarrow\rho}^{(e)} + \left(\sum_{ion} N_{ion} q_{\sigma\rightarrow\rho}^{ion}\right) / N_e$$

Conclusions and opportunities

- Advancing the atomic data required for fusion is still important
- High Z species – calculation of data and development of models underway

- The way atomic data will be used is changing
- Embedded into complex analysis chains, some with machine protection implications (and responsibilities).
- Provenance of atomic data is important
- Validation and assessment must take greater prominence.

- Need to maintain flow of the highest quality data into ADAS
  - Not all data in ADAS is perfect – ideally when faults are found outside the ADAS team an improved dataset would be provided.
- Models must also advance.
- Need more people familiar with using atomic data.
  - Ideally across the ITER domestic agencies
  - Atomic physics and plasma spectroscopy is not a moribund subject

Annual ADAS workshop

ADAS Workshop 2015

The 2015 ADAS Workshop will be held on 1 – 2 October in Catania, Sicily and will be hosted by **INAF — Osservatorio Astrofisico di Catania**.

This year the workshop moves to a Thursday and Friday, with an informal get together on Wednesday 30 September. We hope to have a stronger astrophysics theme than usual. More details in the next few weeks.

References

ADAS : http://adas.ac.uk

ADAS courses : http://www.adas-fusion.eu/courses.php

OPEN-ADAS : http://open.adas.ac.uk

Spectroscopy in JET ILW : J W Coenen et al, Nuclear Fusion, **53** (2013) 073043

Generalized CR model : H P summers et al, Plasma Phys. Control. Fusion, **48** (2006) p263

Beam stopping model : H Anderson et al, Plasma Phys. Control. Fusion, **42** (2000) p781

Lithium GCR : S D Loch et al, Atomic Data and Nuclear Data Tables, **92** (2006) p 813

Lithium excitation : D C Griffin et al, Phys. Rev. A, **64** (2001) 032718

Lithium density dependent rate : J P Allain et al, Nuclear Fusion, **44** (2004) p655

W^{44+} : Awaiting publication and C P Balance et al, J. Phys. B, **40** (2007) p247

W^{18+} dielectronic recombination: K Spruck et al, Phys. Rev. A, **90** (2014) 032715