ADAS: Atomic data, modelling and analysis for fusion

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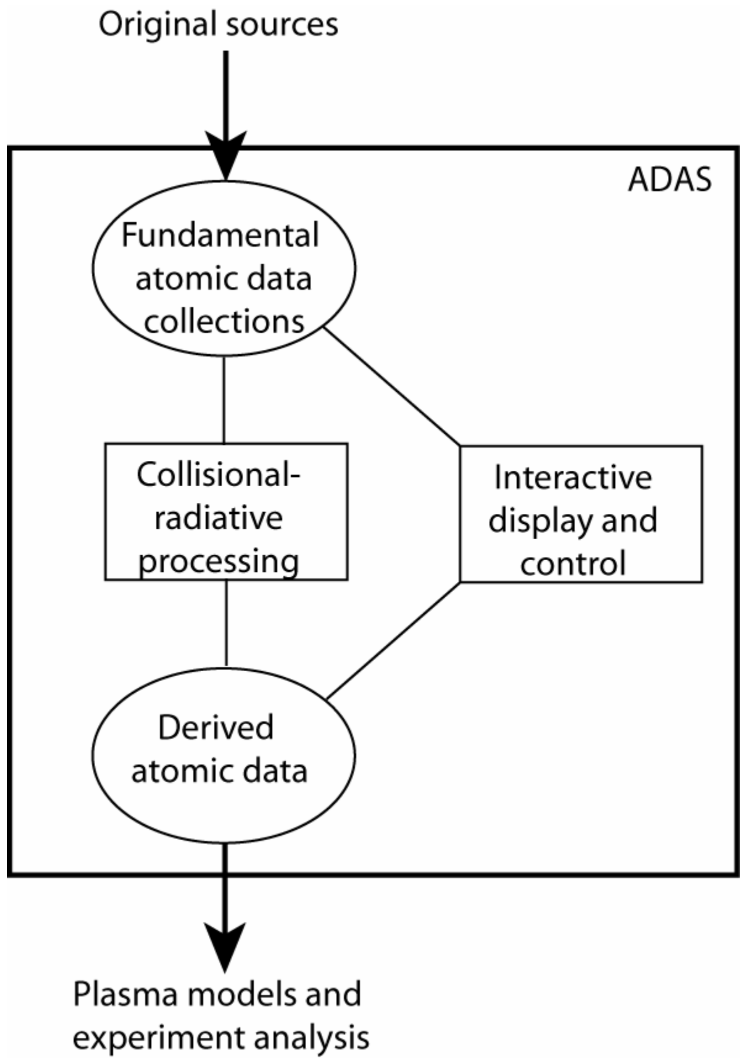
Overview

- The Atomic Data and Analysis Structure, ADAS, is a system of computer codes and data for the support of fusion and astrophysics.
- It originated at the JET Joint Undertaking in 1986 and has operated since 1994 through the ADAS Project.
- The Project is self-funded by its members.
- Most large fusion laboratories are members of the Project.

ADAS modelling schematic



ADAS interactive code series

Interactive codes are grouped in series. Currently ~ 80 codes.

Series	Content	Codes
1	Atomic data entry and verification	8
2	Population processing	16
3	Charge exchange processing	14
4	Recombination, ionisation processing	15
5	General interrogation programs	10
6	Data analysis and spectral fitting	3
7	Creating and using dielectronic data	4
8	Structure and excitation calculations	8

ADAS data formats

- ADAS datasets have precisely defined organisation.
- The are called ADAS data formats (adfs) and there are currently 48 adfs.
- The fundamental and derived database occupies ~ 2.5 Gbyte.

Adf no.	**Content**	**Sub-libraries**	**Files**
adf04	Specific ion data	68(+86)	1078
adf09	State selective dielectronic data	35	1531
adf11	Collisional radiative rec., ion., power coeffts.	40(+86)	344
adf12	Charge exchange effective emission coeffts.	8	45
adf15	Photon emissivity coefficients	17(+86)	173
adf21	Beam stopping coefficients	8	218
adf40	Feature emissivity coefficients	(+86)	2
adf48	State selective radiative recom. Coeffts.	12	660

ADAS subroutine libraries

These provide the practical route for the experienced ADAS user to embed ADAS data or methods within his/her own computations

- There are 1733 subroutines in FORTRAN, 1233 procedures in IDL with smaller numbers in C and MATLAB.

- Of special note are the *xxdata_<nn>* subroutines and procedures which deliver complete dataset contents in a structure to the FORTAN code or IDL command line.

- Wrappers, such as *run_adas408*, provide non-interactively the capabilities of selected interactive codes

Ionisation state and emission of elements

- In fusion, for many years there has been a focus on low-Z elements in plasma-facing wall components, especially He, Li, Be, B, C, N, O and Ne.

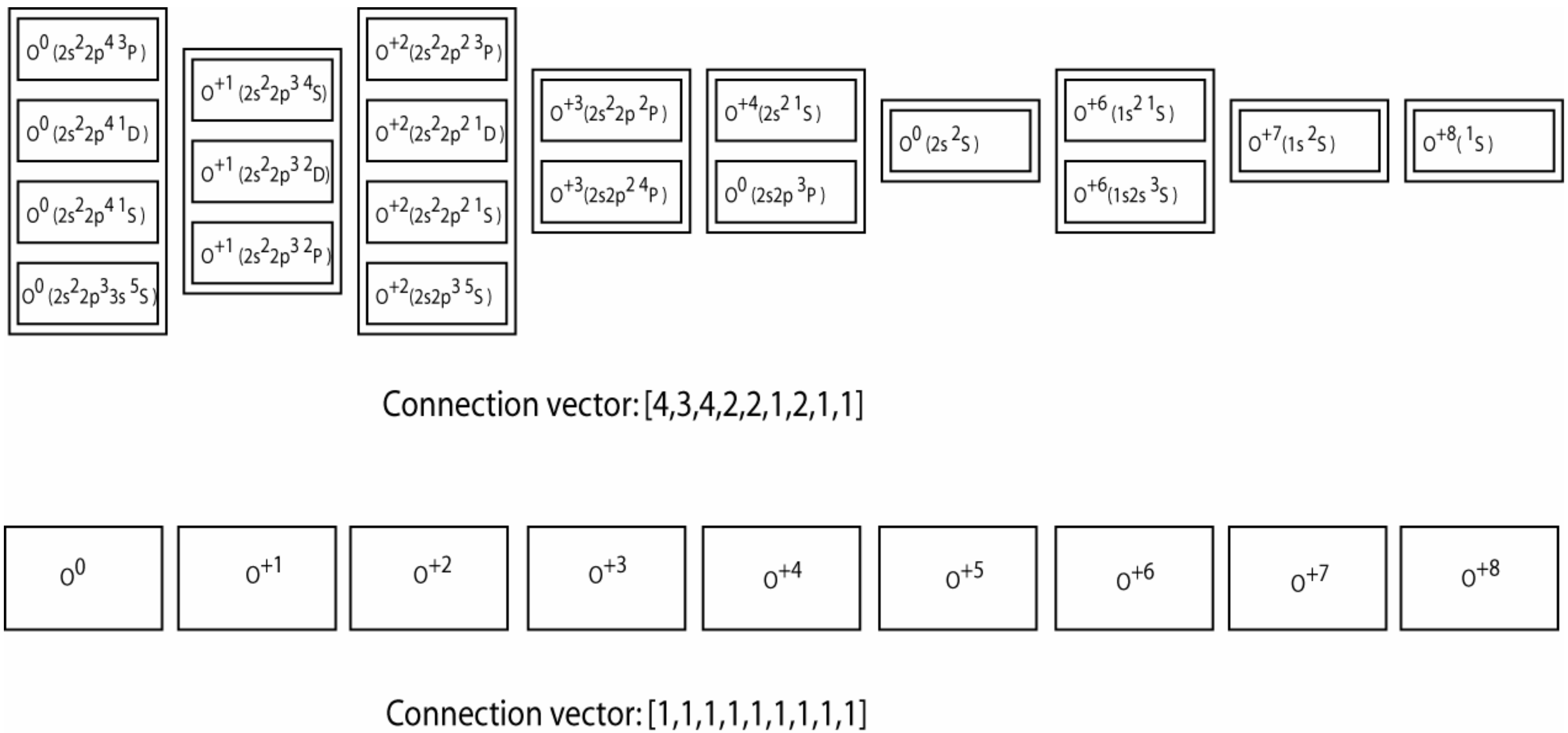
- In turn there has been comprehensive production of the fundamental collision cross-section data required for their modelling in fusion

- The models of the distributions of excited populations and ionisation stages have become sophisticated.

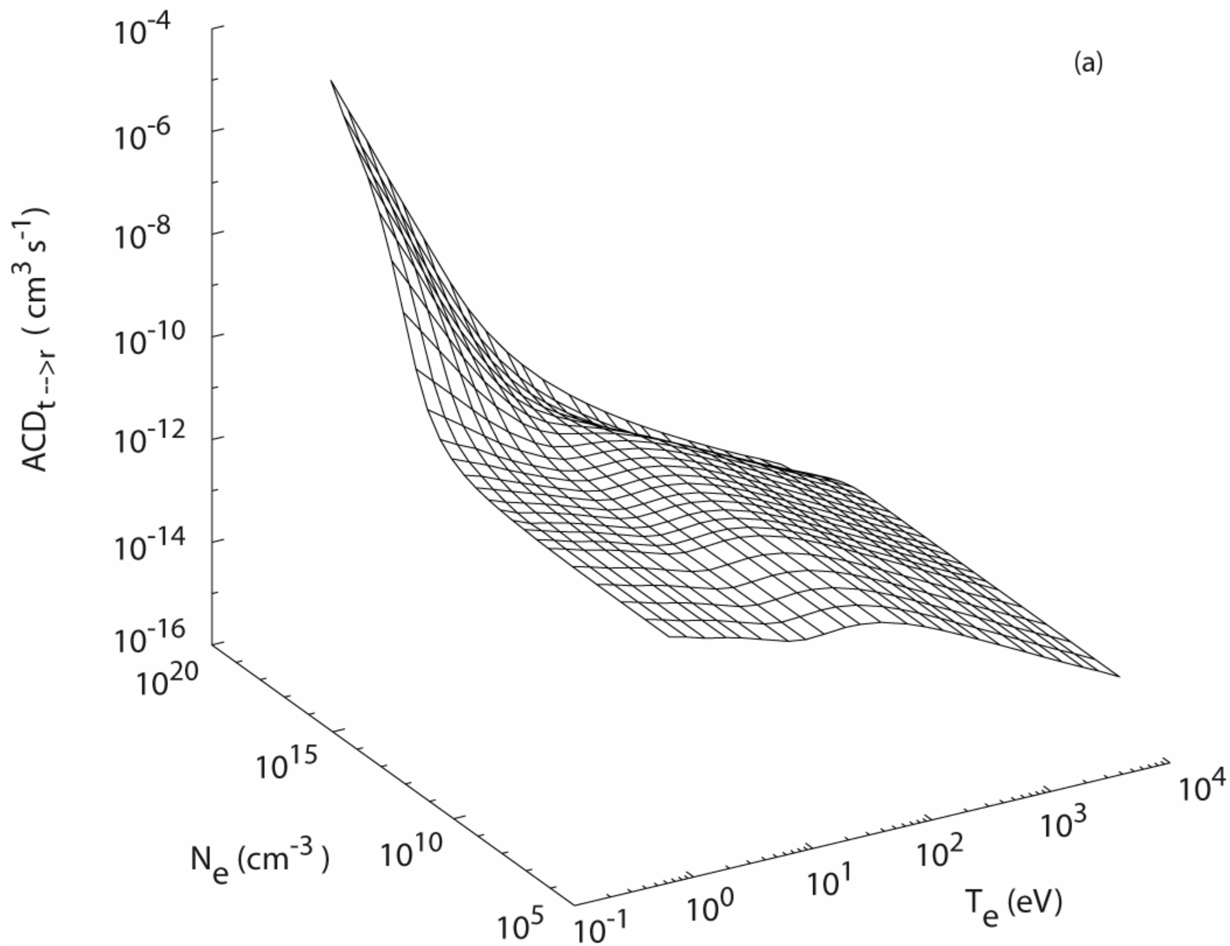
- In ADAS, for light elements, generalised collisional-radiative (GCR) modelling is the norm.

- The detailed emission predictions from such models in the confrontation with spectroscopic observations has in large measure been successful.

Metastables of oxygen used in ADAS for generalised collisional-radiative modelling



Generalised collisional-radiative recombination coefficients

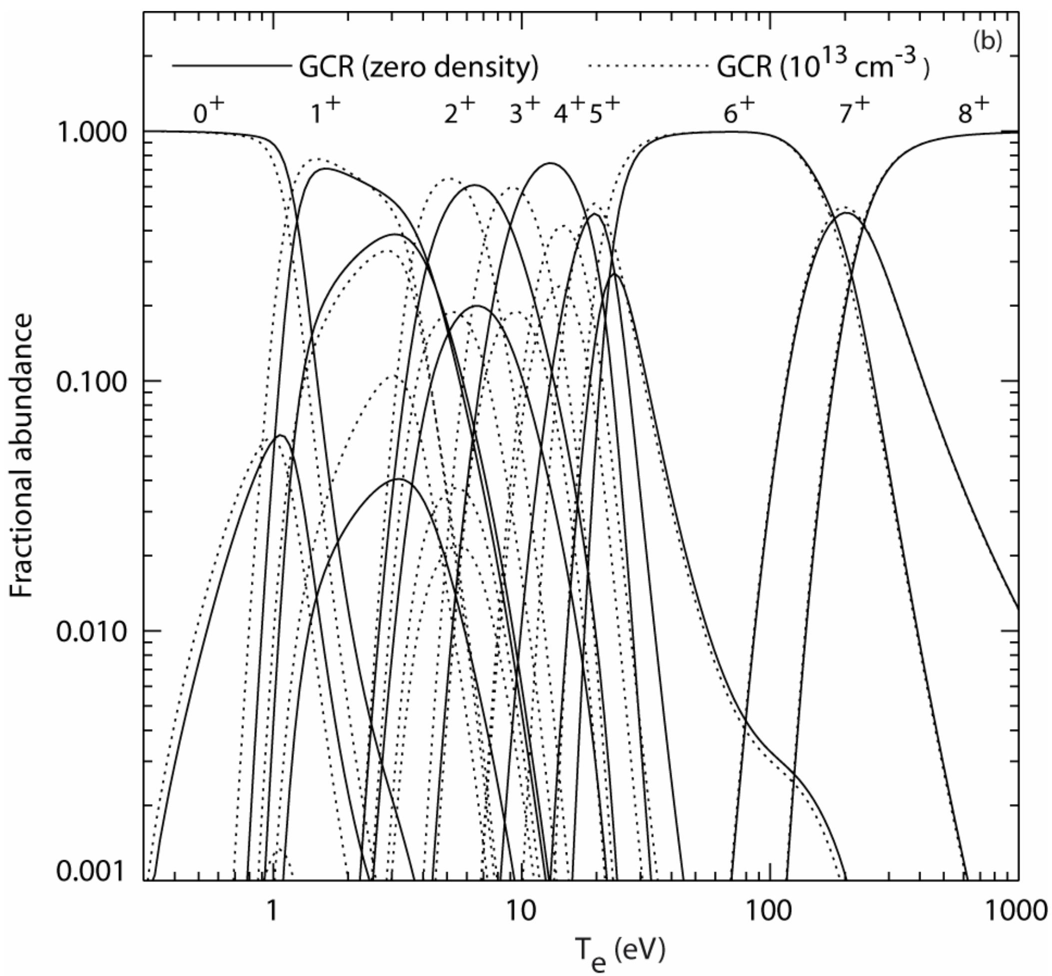


O^{+4} + e → O^{+3}

ACD (2s2p ^3P → 2s2p^2 ^4P)

Data from ADAS data format *adf11, year number 96*, sub-library acd96r

Equilibrium fractional abundances of oxygen metastables from the GCR picture

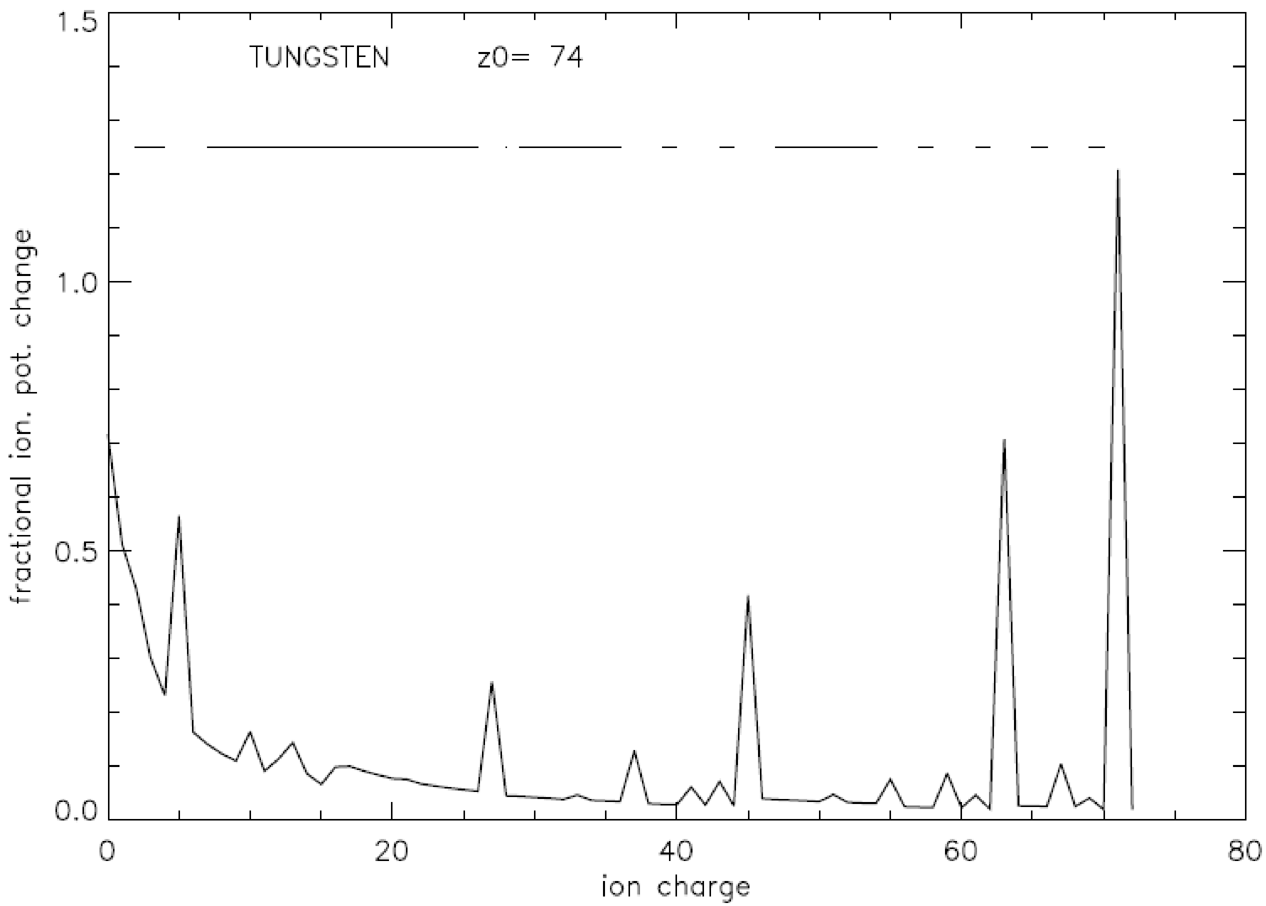


Generated using run_adas405

Heavy atomic species and ITER

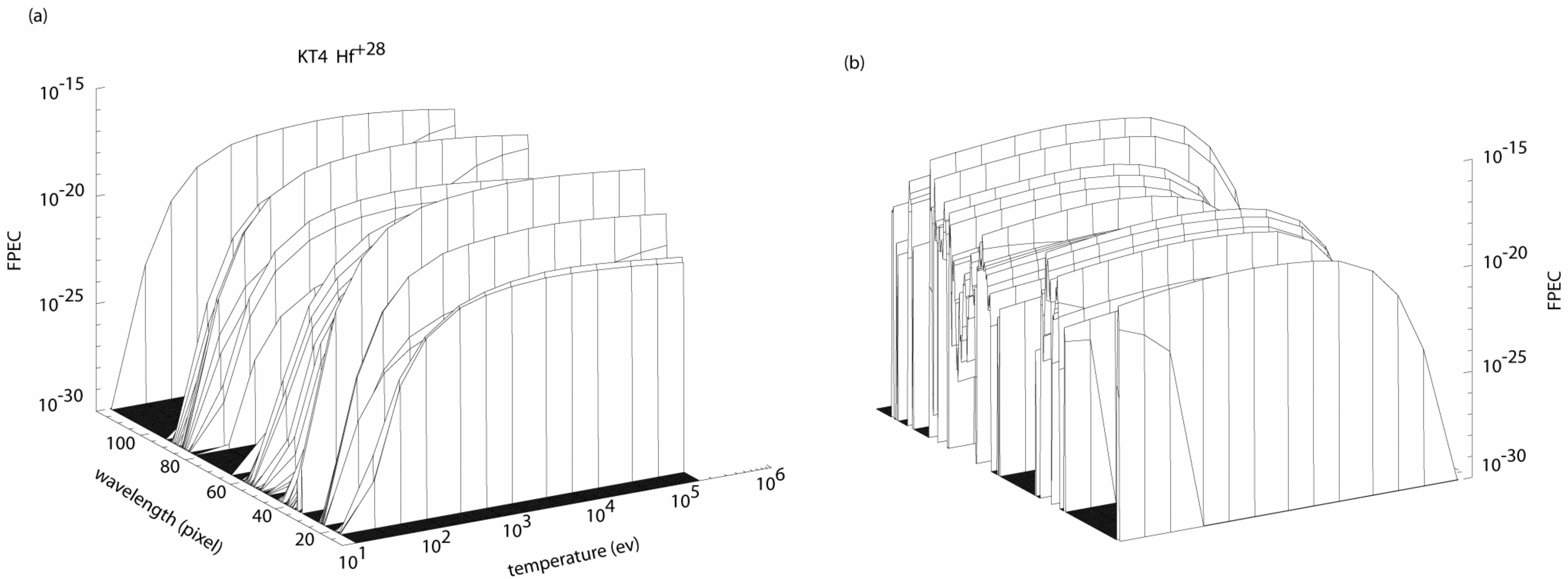
- ITER measurement requirements for plasma facing and structural components span Be, C and W.
- Additional seeded impurities for diagnostics and control include Ne, Ar and Kr. Also of course He is present.
- Possibly other structural elements such as Cr, Ni, Cu, Mo
- Possibly various medium/heavy species as (erosion) markers (Sn, Ag, Au, …).

Fractional change in ionisation potential for tungsten ions



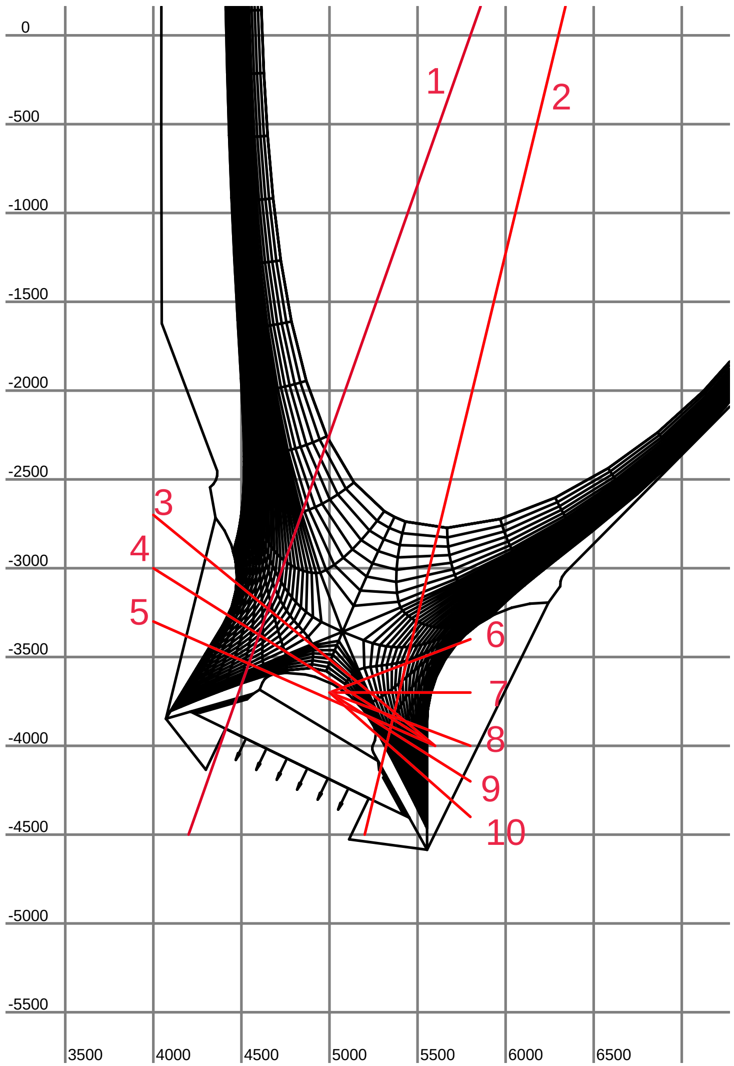
Data from ADAS data format *adf00*.

FPEC for Hf^{+28} in the spectral range of the XUV ('SOXMOS' - KT4) spectrometer at JET Vs T_e. $N_e = 5.0 \times 10^{+13}$ cm^{-3}.



FPEC data archived in ADAS data format *adf40*, extracted by ADAS code *read_adf40.pro*

Expected ITER lines of sight for use in predictive analysis



ITER plasma simulations and lines of sight

Three scenarios

Different power loading on the divertor:

(1) high power of 13 MW/m^2

(2) intermediate power 5 MW/m^2

(3) partially detached plasma with 2 MW/m^2

These correspond to simulations #882, #844 and #899.

Selected chords

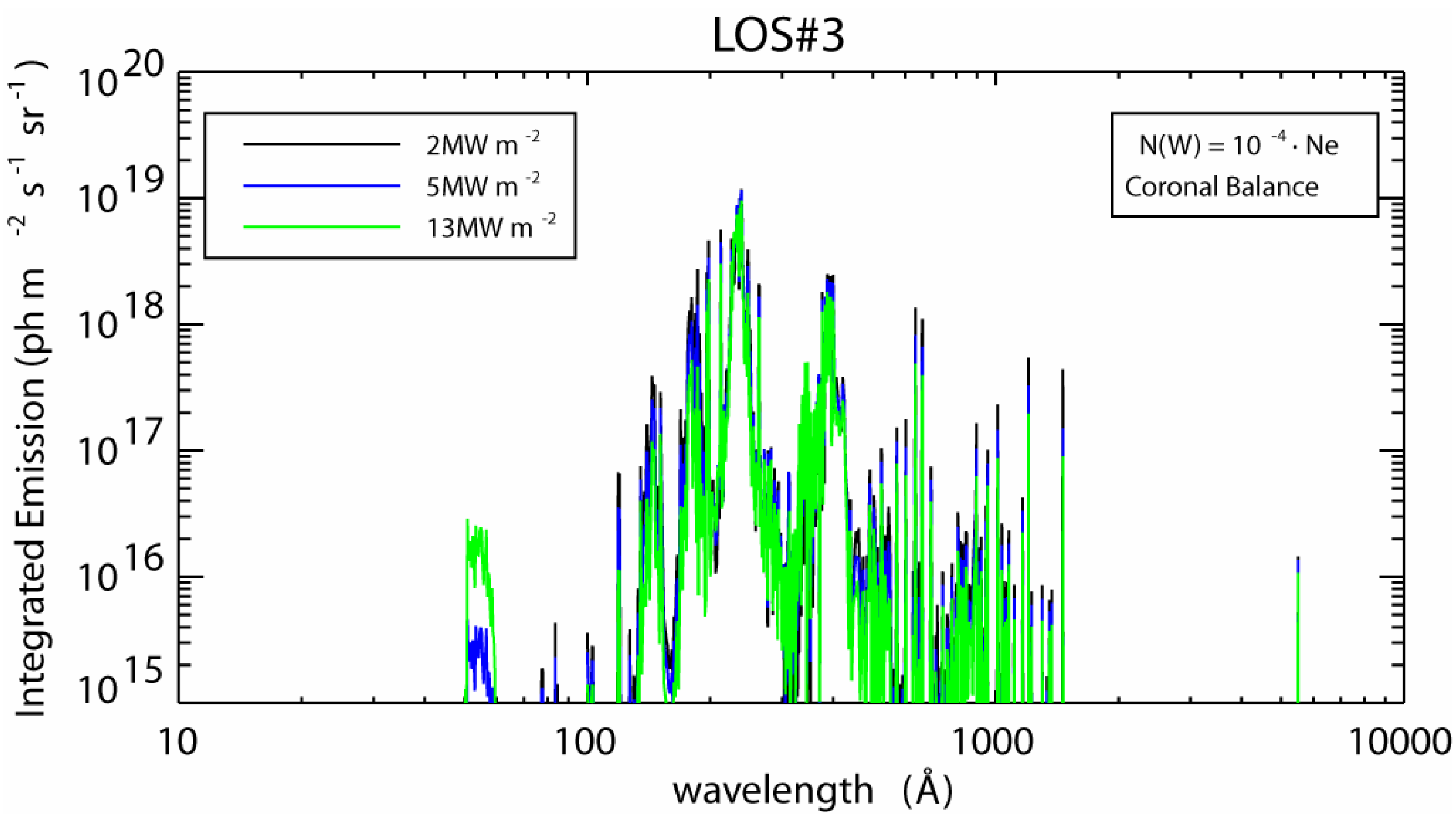
#3, #4 and #5 see both divertor legs.

Fan of chords (#6-#10) view the wall of the outer divertor leg.

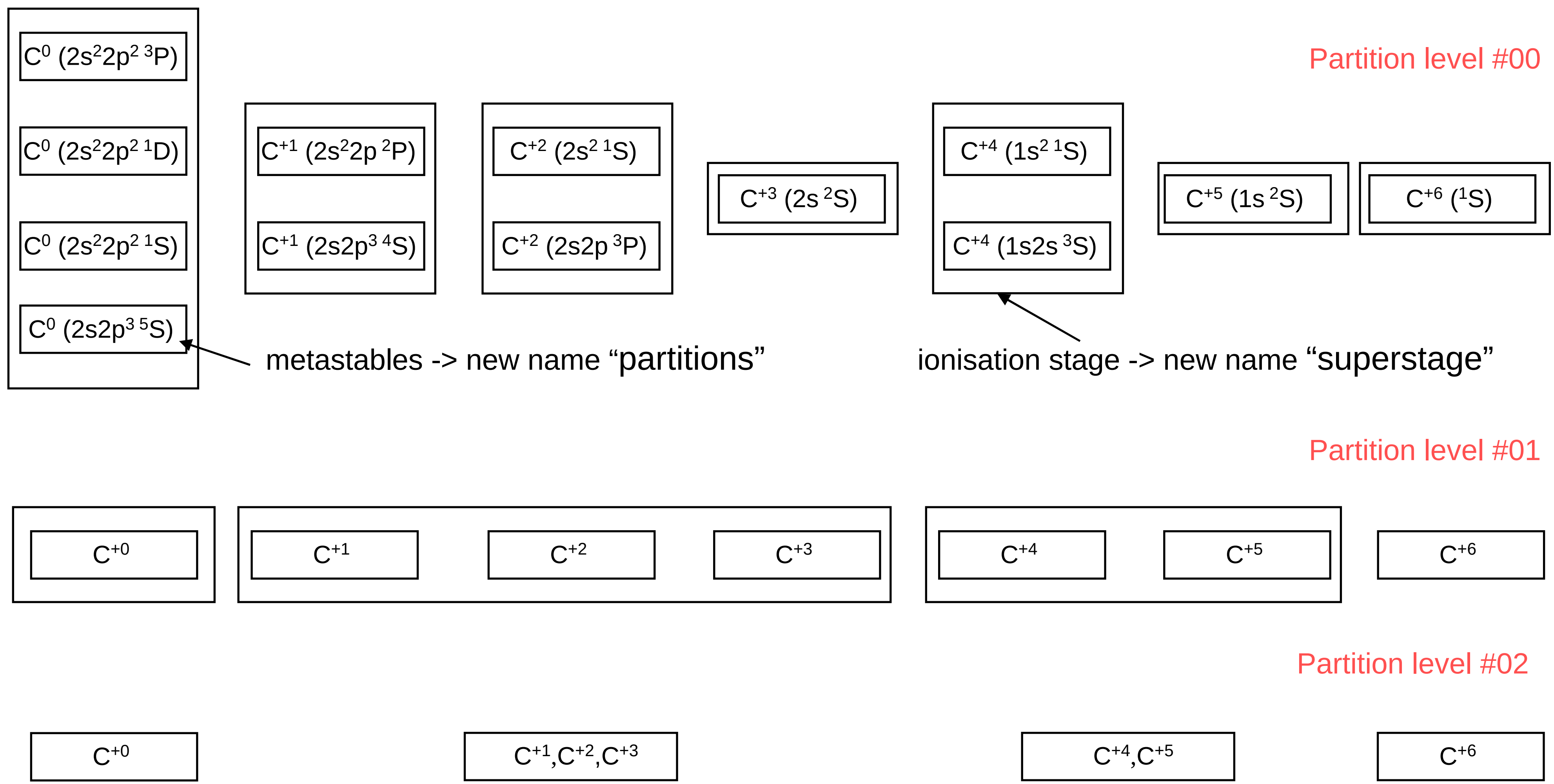
#1 and #2 view each leg but see all of the confined core plasma as well.

B2-Eirene background plasma simulations in poloidal magnetic-field based grid shown.

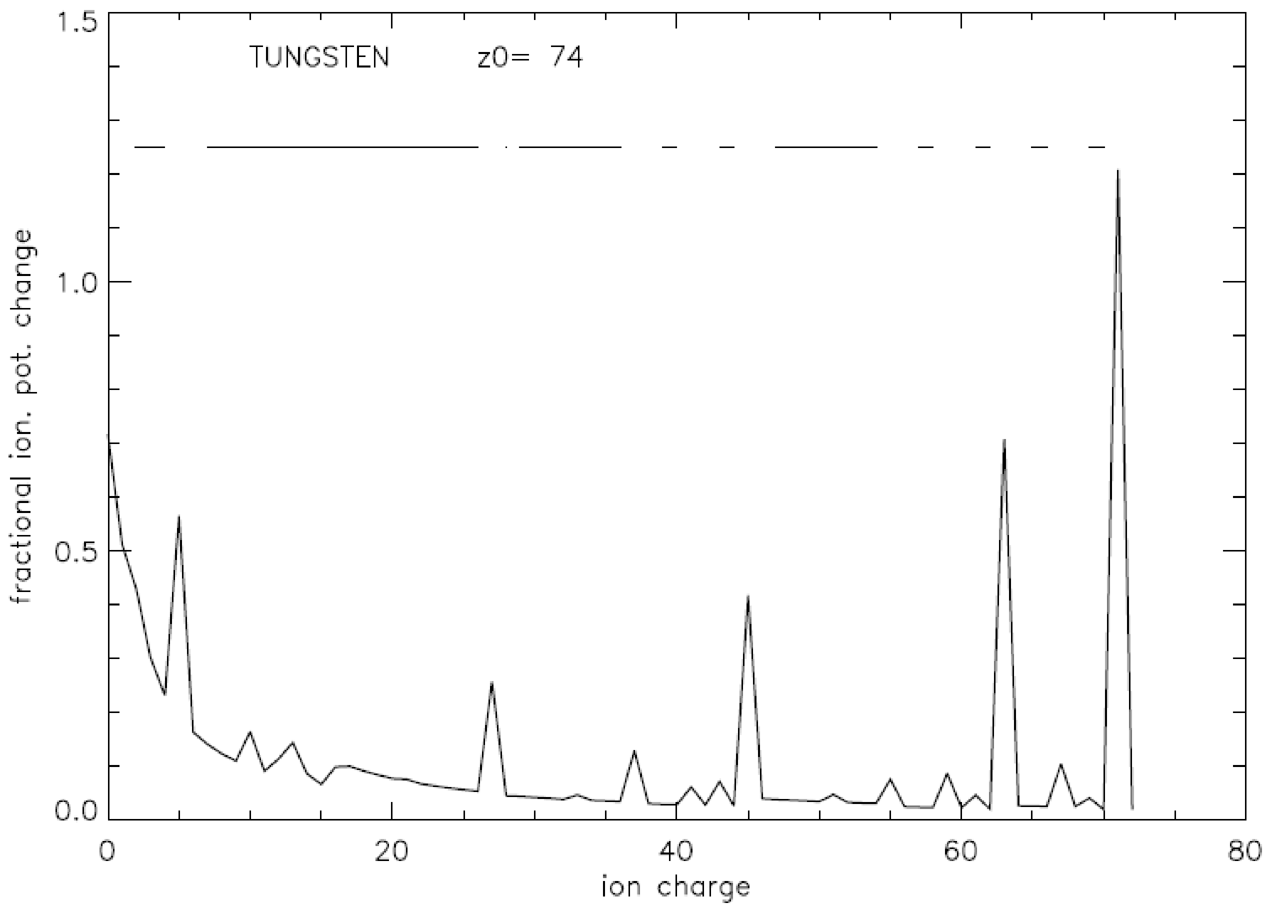
The integrated emission from tungsten for lines of sight which view both legs of the divertor. Coronal balance and a tungsten concentration of $10^{-4} \times N_e$ are assumed.



Superstages
carbon as an illustration

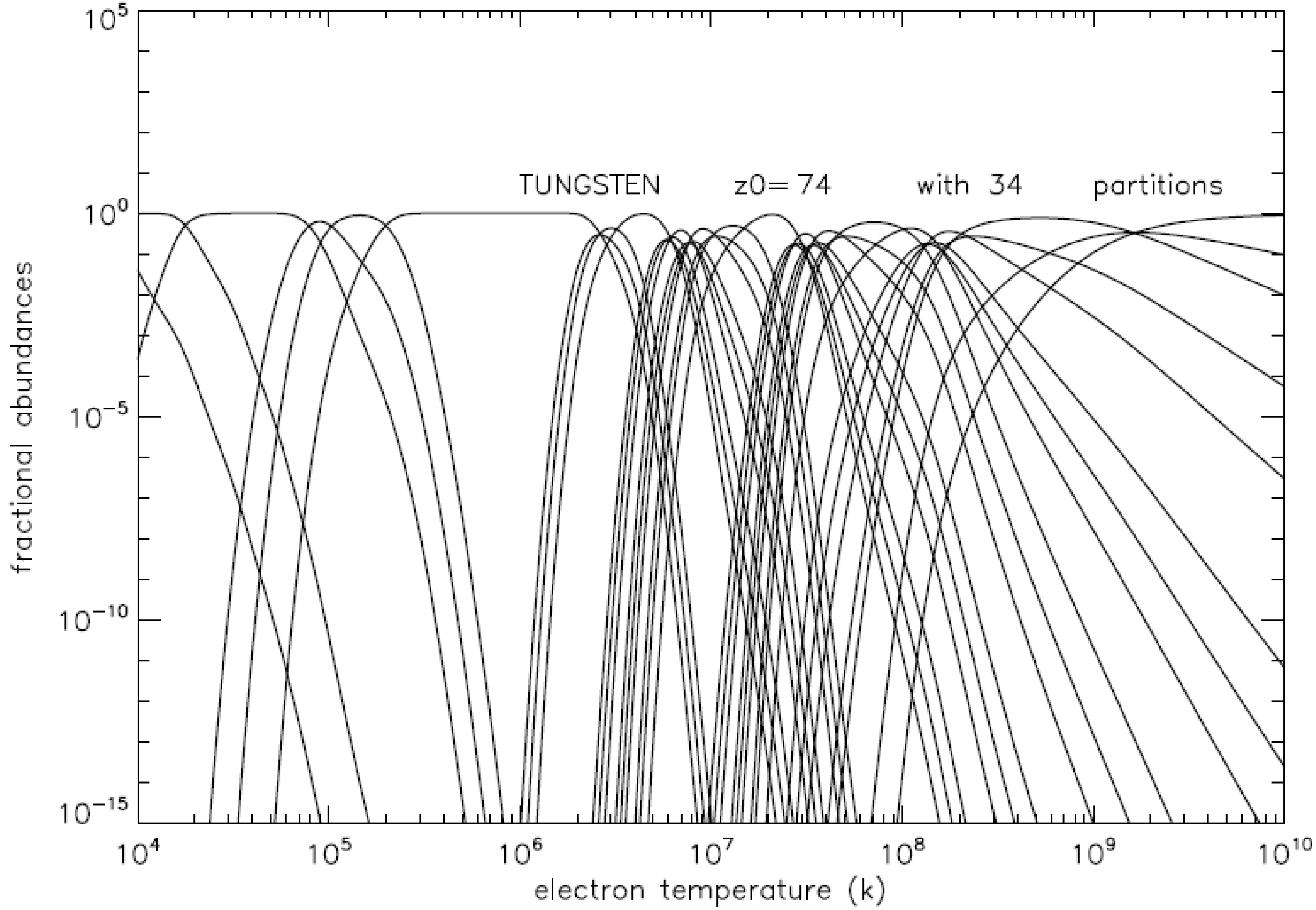


The natural partition for tungsten



Data from ADAS data format *adf00*.

Natural partition ionisation balance for tungsten



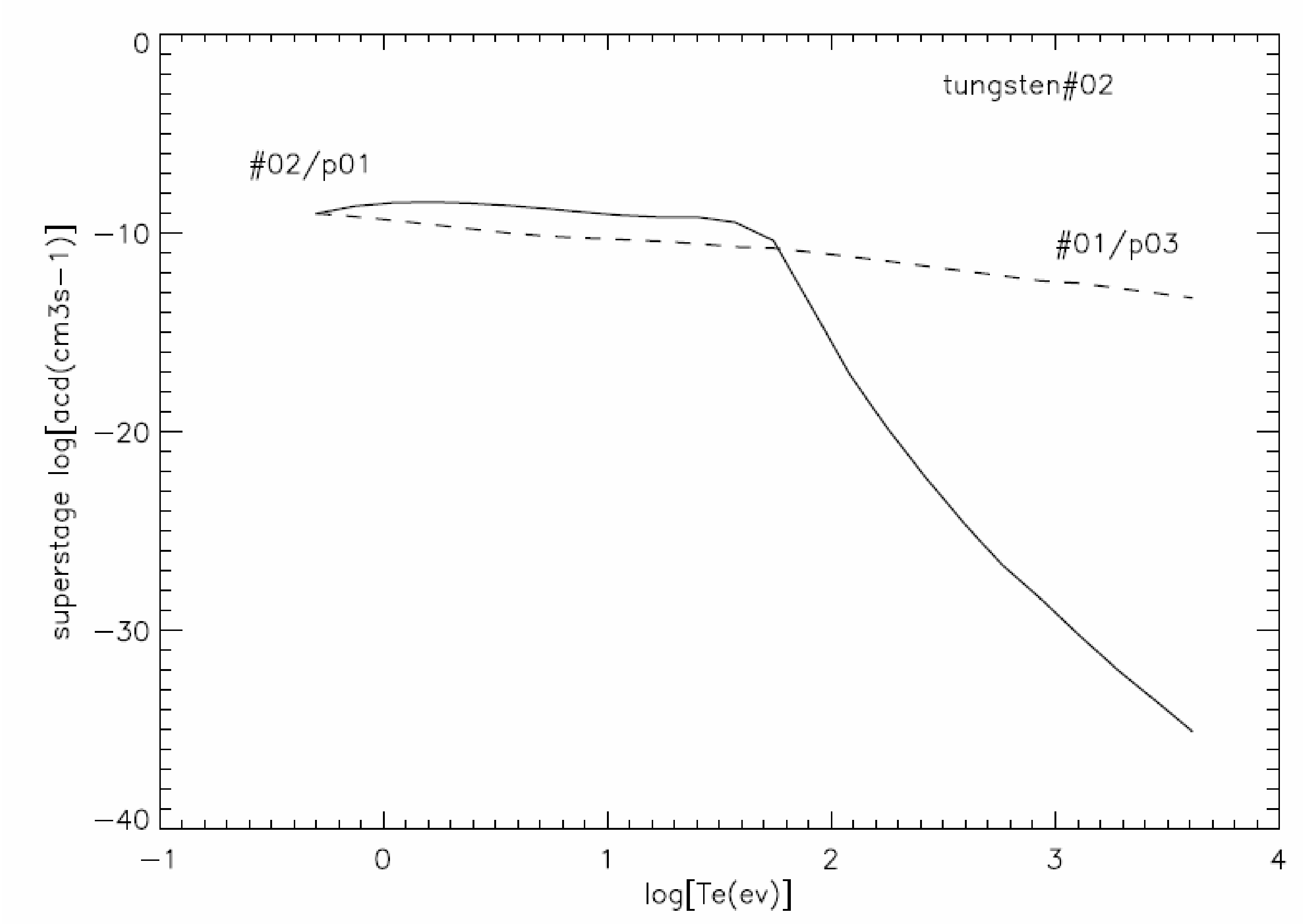
Ionis./recom data archived in ADAS data format *adf11*, extracted, processed and displayed by ADAS code *ADAS405*

Aggressive tungsten bundling for 2-D and 3-D divertor transport models (#02 partition)

Superstages

p00	p01	p02	p03	p04	p05	p06
W^{+0}	W^{+2}	W^{+6}	W^{+13}	W^{+28}	W^{+46}	W^{+56}
W^{+1}	W^{+3}	W^{+7}	W^{+14}	W^{+29}	W^{+47}	W^{+57}
	W^{+4}	W^{+8}	W^{+15}	W^{+30}	W^{+48}	W^{+58}
	W^{+5}	W^{+9}	W^{+16}	W^{+31}	W^{+49}	W^{+59}
		W^{+10}	W^{+17}	W^{+32}	W^{+50}	W^{+60}
		W^{+11}	W^{+18}	W^{+33}	W^{+51}	W^{+61}
		W^{+12}	W^{+19}	W^{+34}	W^{+52}	W^{+62}
			W^{+20}	W^{+35}	W^{+53}	W^{+63}
			W^{+21}	W^{+36}	W^{+54}	W^{+64}
			W^{+22}	W^{+37}	W^{+55}	W^{+65}
			W^{+23}	W^{+38}		W^{+66}
			W^{+24}	W^{+39}		W^{+67}
			W^{+25}	W^{+40}		W^{+68}
			W^{+26}	W^{+41}		W^{+70}
			W^{+27}	W^{+42}		W^{+71}
				W^{+43}		W^{+72}
				W^{+44}		W^{+73}
				W^{+45}		W^{+74}

Effective superstage recombination coefficient for tungsten #02 partition

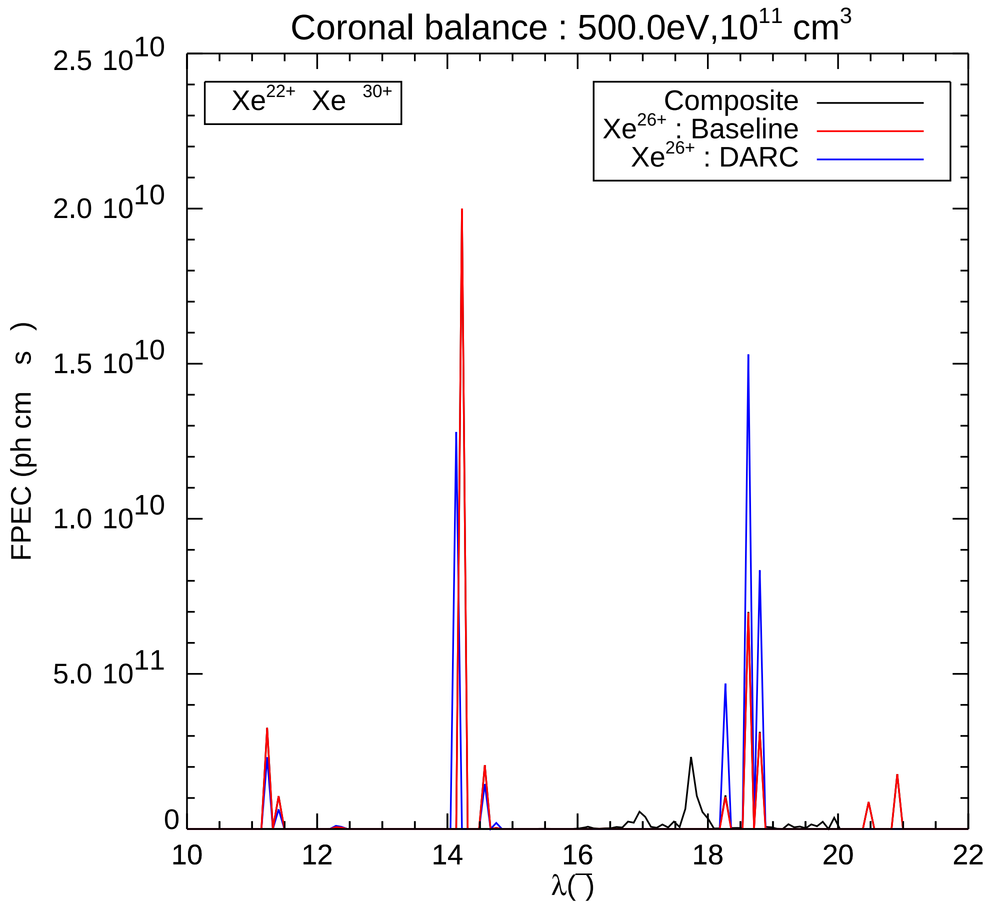


Superstage data prepared by ADAS code ADAS416 and archived in ADAS data format *adf11, adf15, adf40*

adf11 sub-classes for application

ADF11 Subclass	Character	Basic	Full GCR	Superstage
ACD	effective recombination coefft.	x	x	x
SCD	effective ionisation coefft.	x	x	x
CCD	effective CX recom. coefft.	(x)		(x)
PLT	effective excit. power coefft.	x	x	x
PRB	effective recom./brems. power coefft.	x	x	x
PRC	CX recom. power coefft.	(x)		(x)
QCD	effective metas. coupling coefft.		x	
XCD	effective parent metas. coupling coefft.		x	
ZCD	effective superstage charge			x
YCD	effective superstage squared charge			x
ECD	effective ionisation potential			x
ADF15 Subclass	**Character**			
$PEC^{(exc)}$	excit. photon emiss. coefft.	x	x	x
$PEC^{(rec)}$	recom. photon emiss. coefft.		x	
$FPEC^{(exc)}$	feature excit. photon emiss. coefft.			x
$FPEC^{(rec)}$	feature recom. photon emiss. coefft.			

Xenon and spectral emission
Precision in the key lines of the spectrum



Spectral emission in the 10-12 A region. The emission is assembled from the baseline feature photon emissivity coefficients of each ionisation stage and combined with the ionisation balance at T_e=500eV and N_e=10^{11}cm^{-3}.
The emission of the Xe^{+26} stage is shown in red.
The effect of including the feature photon emissivity coefficient from the GRASP/DARC calculation is shown in blue.
Note that the familiar lasing line in this ion, $Xe^{+26}(3d^{10}\ ^1S_0$ - $3d^9 4p\ ^1P_1)$ is at 99.6 A.

Extension of the scope of the ADAS project (Fundamental data)

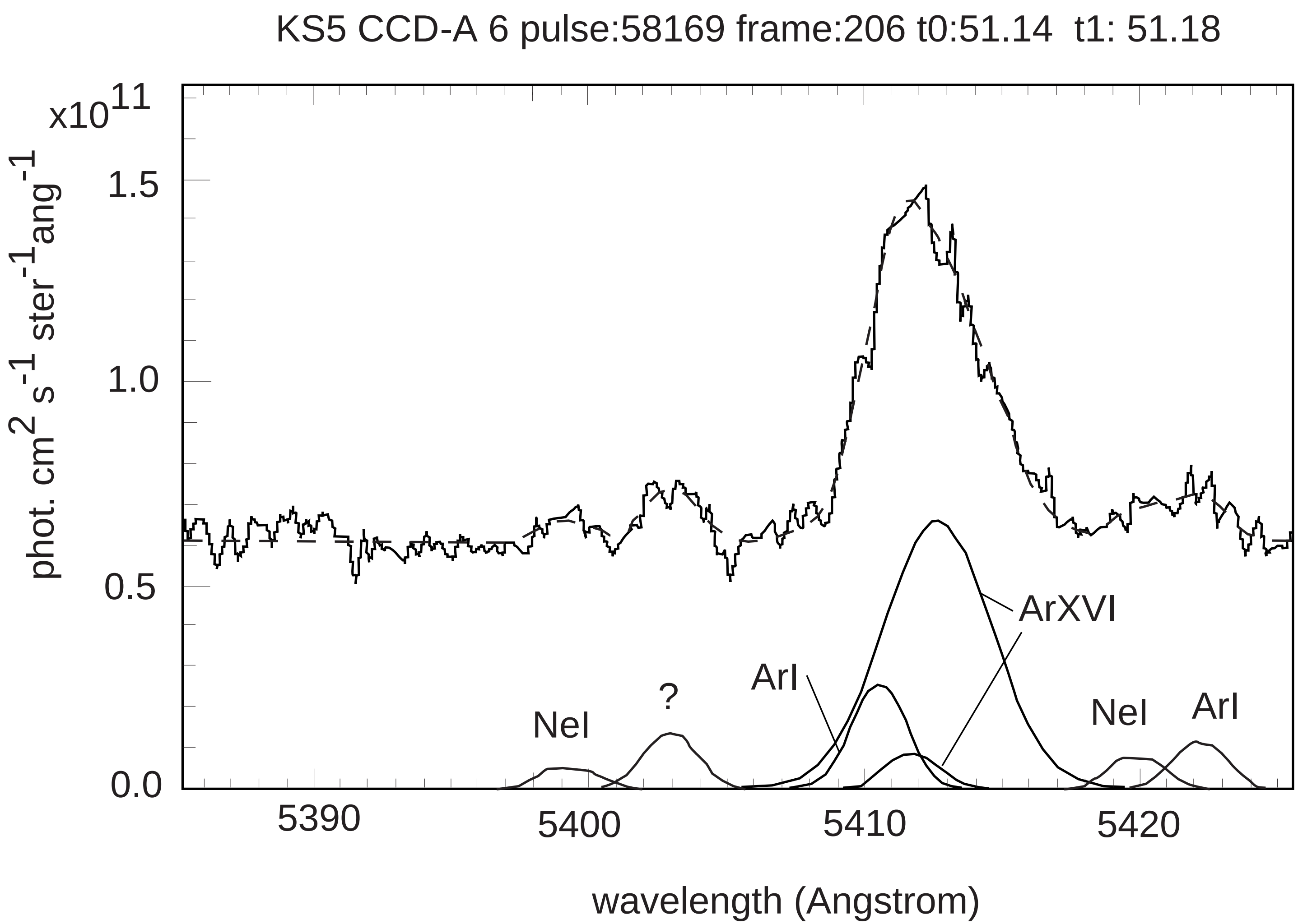
- It has been evident for some years that ADAS cannot live entirely within its original ‘local’ atomic modelling boundaries.
- The ADAS Project and it spin-off projects now put great effort into procuring and generating its own fundamental data.
- Offline-ADAS was initiated some time ago to this end with complex codes, designed for scripted running on large/parallel machines including:
  - State selective dielectronic data (adf09 – adas7#1)
  - Complete heavy species baseline (adf04, adf15, adf40 - adas8#1)
  - Ionisation cross-section data for heavy species (adf07,adf23 – adas8#2)
  - Automatic R-matrix calculations along iso-electronic sequences (adf04 – adas8#3)
- Targetted atoms and ions.

Extension of the scope of the ADAS project (Integrated diagnostic applications)

- Impurity transport codes
  - SANCO (Martin O'Mullane)
- Analysis code development
  - CXSFIT (Charge exchange spectral interval fitting)
  - NEW-CHEAP (Integrated charge exchange emission analysis package)
  - UTC (Universal transport analysis package)
- Special feature analysis
  - MSE/BES etc.

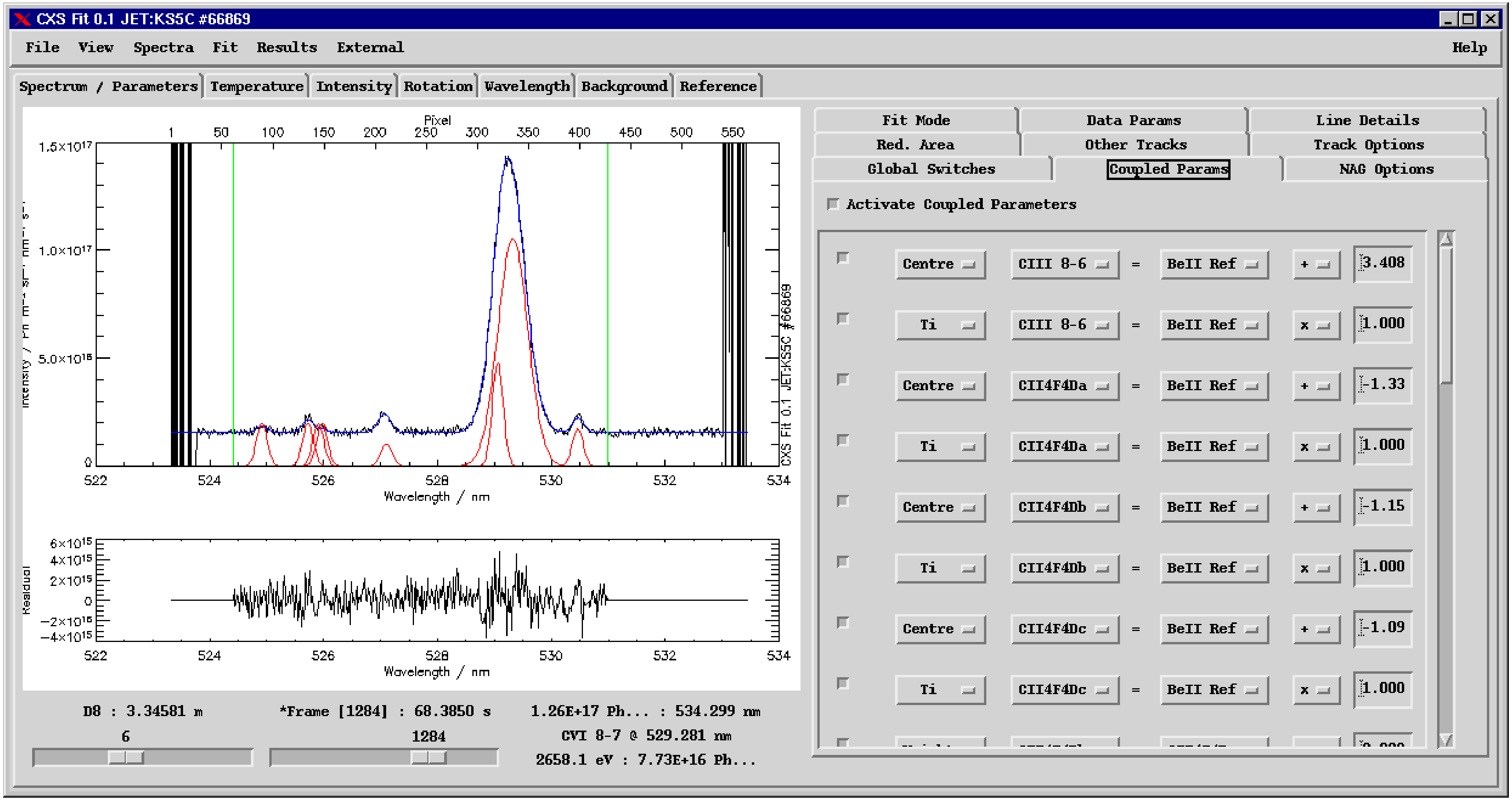
These constitute shared developments between a number of (European/Japan/USA) partners for collaborative use and analysis on a range of tokamaks/stellarators and in preparation for ITER. Code development is done by the ADAS team and the codes are maintained along with main ADAS.

Charge exchange analysis

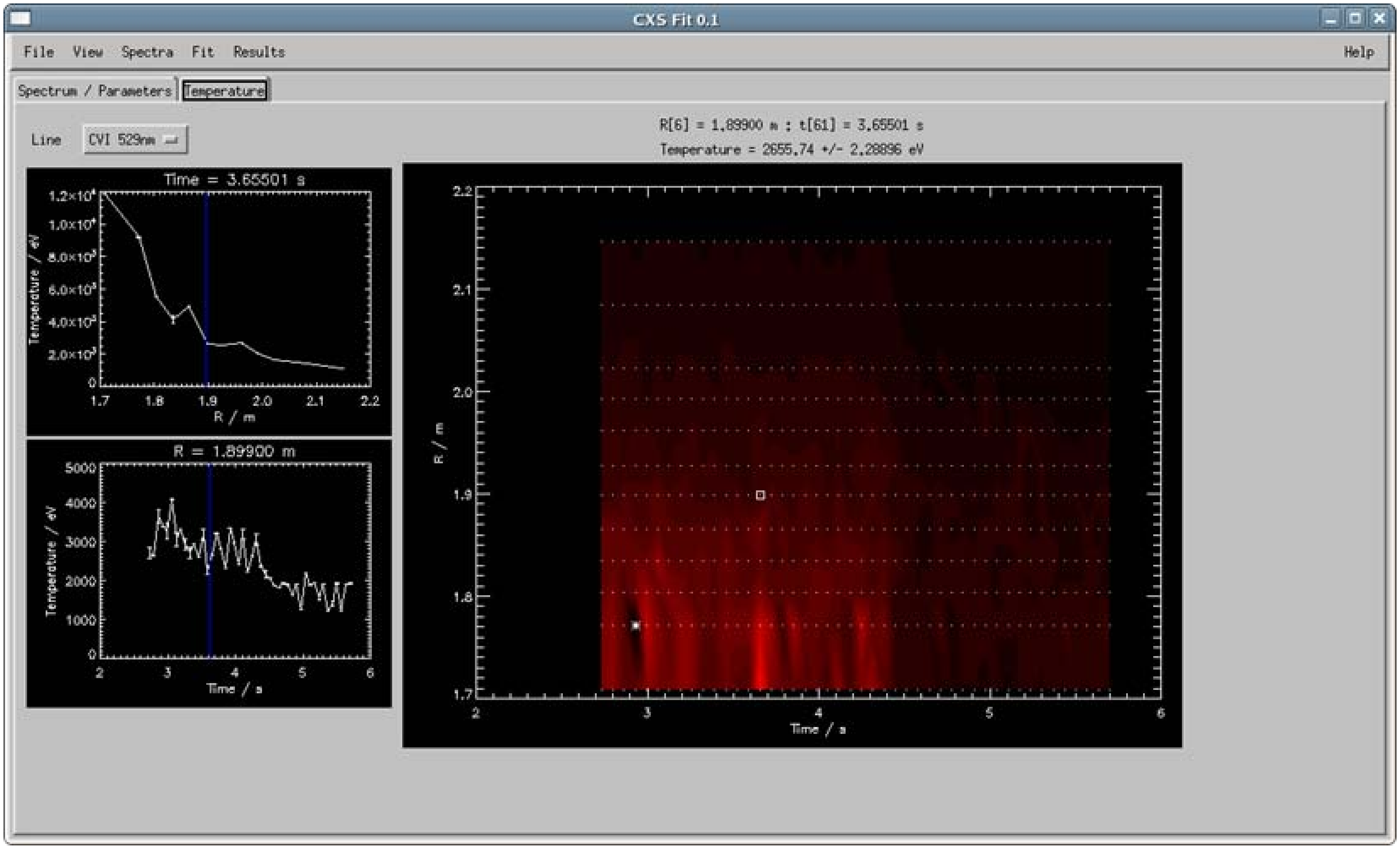


ArXVI(n=15-14)

CXSFIT


CXS Fit 0.1 JET:KS5C #66869
File View Spectra Fit Results External Help
Spectrum / Parameters
Temperature
Intensity
Rotation
Wavelength
Background
Reference
Fit Mode
Data Params
Line Details
Red. Area
Other Tracks
Track Options
Global Switches
Coupled Params
NAG Options
Activate Coupled Parameters
Centre CIII 8-6 = BeII Ref + 3.408
Ti CIII 8-6 = BeII Ref x 1.000
Centre CII4F4Da = BeII Ref + -1.33
Ti CII4F4Da = BeII Ref x 1.000
Centre CII4F4Db = BeII Ref + -1.15
Ti CII4F4Db = BeII Ref x 1.000
Centre CII4F4Dc = BeII Ref + -1.09
Ti CII4F4Dc = BeII Ref x 1.000
Pixel
Wavelength / nm
Residual
D8 : 3.34581 m
*Frame [1284] : 68.3850 s
1.26E+17 Ph... : 534.299 nm
CVI 8-7 @ 529.281 nm
2658.1 eV : 7.73E+16 Ph...

CXSFIT



CXS Fit 0.1
File View Spectra Fit Results
Help
Spectrum / Parameters
Temperature
Line
CVI 529nm
R[6] = 1.89900 m : t[61] = 3.65501 s
Temperature = 2655.74 +/- 2.28896 eV
Time = 3.65501 s
Temperature / eV
R / m
R = 1.89900 m
Temperature / eV
Time / s
R / m
Time / s

ADAS availability and dissemination

- ADAS is a provision for the laboratories which are its sponsors. All persons and visitors at these sites have access to ADAS. There is central provision at EFDA-JET accessible from all Associated Laboratories of the European fusion programme.
- There is access through data centres at Oak Ridge National Data Centre, USA and the National Institute for Fusion Science, Japan.
- Of the ~2.5 Gbyte of ADAS data, ~1.5 Gbyte is public domain, ~150 Mbyte of key adf11 and adf15 data are supplied freely with transport models from IPP-Garching since 1998.
- Under the joint sponsorship of the IAEA Atomic and Molecular Data Unit, Vienna and the ADAS Project, an initiative is underway to give access to selected ADAS data and facilities via the IAEA website – called OPEN-ADAS.
- A new tagging, index and search system is being developed for the principal ADAS data formats to enable identification of appropriate data for applications and to provide guidance on the use of the data. The tagging of ADAS data is being expanded to support this.
- Sets of procedures for download, along with the data themselves are being provided in a number of languages for reading ADAS data into a user's own code.

OPEN-ADAS

ADAS
Atomic Data and Analysis Structure

OPEN-ADAS Version 0.1B
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- Search by ion
- Search by data class
- Documentation
- Online codes
- Download codes
- About ADAS

ADF04 | ADF08 | ADF09 | ADF11 | ADF12 | ADF15 | ADF40

ADF15 Search Results

Wavelength
Minimum (Å) 2000
Maximum (Å) 5000

Ion
Element c
Element symbol or atomic number (e.g. C or 6)

Resolve Results By
- (•) Transition (longer list)
- ( ) File (shorter list)

Search for ADF15 Files

Wavelength	Ion	Transition	File Details
2274.6Å	C^{4+}	$^{3}P_{4.0} \rightarrow {}^{3}S_{1.0}$	pec93#c_pjr#c4.dat
2274.7Å	C^{4+}	1S1 2P1 $^{3}P_{4.0} \rightarrow$ 1S1 2S1 $^{3}S_{1.0}$	pec96#c_pju#c4.dat
2274.7Å	C^{4+}	1S1 2P1 $^{3}P_{4.0} \rightarrow$ 1S1 2S1 $^{3}S_{1.0}$	pec96#c_pjr#c4.dat
3527.7Å	C^{4+}	$^{1}P_{1.0} \rightarrow {}^{1}S_{0.0}$	pec93#c_pjr#c4.dat

Comments and questions to: adas@phys.strath.ac.uk

OPEN-ADAS

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Atomic Data and Analysis Structure

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ADF04 | ADF08 | ADF09 | ADF11 | ADF12 | ADF15 | ADF40

ADF15 File: pec96#c_pju#c4.dat

Ion: C^{4+}
Temperature Range: 1.08 → 6460 eV
Density Range 781000 → 7.81e+19 cm^{-3}
Filename: pec96#c_pju#c4.dat
Full Path: adf15/pec96#c/pec96#c_pju#c4.dat
MD5SUM: 0c9903fb467e4fd5de16561cc02ba5c6

Download Options
Download Data
Documentation
Software libraries

Show origin information

Wavelength	Transition	Type	Driving Population
32.8Å	1S1 5D1 $^1D_{2.0} \rightarrow$ 1S2 $^1S_{0.0}$	Excitation	
32.8Å	1S1 5P1 $^3P_{4.0} \rightarrow$ 1S2 $^1S_{0.0}$	Excitation	
32.8Å	1S1 5P1 $^1P_{1.0} \rightarrow$ 1S2 $^1S_{0.0}$	Excitation	
32.8Å	1S1 5D1 $^1D_{2.0} \rightarrow$ 1S2 $^1S_{0.0}$	Recombination	
32.8Å	1S1 5P1 $^3P_{4.0} \rightarrow$ 1S2 $^1S_{0.0}$	Recombination	
32.8Å	1S1 5P1 $^1P_{1.0} \rightarrow$ 1S2 $^1S_{0.0}$	Recombination	
32.8Å	1S1 5D1 $^1D_{2.0} \rightarrow$ 1S2 $^1S_{0.0}$	Charge Exchange	
32.8Å	1S1 5P1 $^3P_{4.0} \rightarrow$ 1S2 $^1S_{0.0}$	Charge Exchange	
32.8Å	1S1 5P1 $^1P_{1.0} \rightarrow$ 1S2 $^1S_{0.0}$	Charge Exchange	

Co-workers

Nigel Badnell	(Strathclyde)
Mike Witthoeft	
Adam Foster	
Paul Bryans	(Columbia)
Mitch Pindzola	(Auburn)
Stuart Loch	
Don Griffin	(Rollins)
Connor Ballance	
Thomas Putterich	(ASDEX-U)
Robin Barnsley	(ITER)