ADAS-EU R(13)SU01

ADAS-EU
ADAS for fusion in Europe

Grant: 224607

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ECWP2: Electron Collision Working Party Report 2

20 Dec 2013

Workpackages : 4-2, 5-1, 5-2, 5-3, 27-1*, 27-2*, 28-1* and 28-2*

Category : DRAFT – CONFIDENTIAL

ECWP2: Electron Collision Working Party
Report 2

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Abstract: *The Electron Collision Working Party was an orginal objective of the ADAS-EU project, to be led by Dr. Allan Whiteford. The unexpected departure of Dr. Whiteford from the the Project caused a delay in establishing the working party. In Oct. 2010, Professor Nigel Badnell joined the project and it was possible to restart the Electron Collision Working Party in expert hands. This report summarises activities from Jan. 2012 to Dec 2012.*

Contents

Chapter 1

Introduction

As discussed in report ECWP1, the completion of the primary set of sub-contracts at the end of the second period presented, in the electron collision area, some surprises for the Electron Collision Working Party (ECWP). Thus the measurements on dielectronic recombination (DR) at Justus-Liebig University (see ECWP1 section 2.3) initiated an exploration of very large threshold contributions to the recombination for adjacent ions to W^{+20} (the target of the first study) both theoretically and experimentally and revision of the historical practice of treating low temperature and high temperature DR as essentially orthogonal. This is only one part of the DR problem for fusion. For complex ions, the amount of data to be archived in ADAS and manipulated for generalised-collisional-radiative (GCR) modelling, as practised for light element ions, becomes prohibitive. In report ECWP1, some description was given of the *bbgp* approach developed for ADAS-EU. Another method for condensing the data burden has been developed, called the *hybrid* method. Work on these aspects of DR in period 3 are described in section 2.1 of this report. Also in ECWP1, the new *distorted wave* collision cross-section capability of AUTOSTRUCTURE was described. Large scale exploitation of this method was made in period 3 - see in particular SCIENCE8 section 2.1. The ECWP has been keen to refine these calculations (see SCIENCE8 section 2.4.1) for neutral and near-neutral middle-weight and heavy atoms. Section 2.2 presents some details of the refinement process. The last objective (see section 2.3) has been to merge the atomic structure approaches of Mons-Hainaut (adjusted Cowan) and Vilnius (Jucys approach) with ADAS (AUTOSTRUCTURE). Since AUTOSTRUCTURE (*DW*) is the new level 1 base reference method for ADAS and RMATRIX the top-level selective method for ADAS, it is hoped by such merging to take the high precision Mons-Hainaut and Vilnius atomic structures into the collisional domain. This goal is not yet achieved, but progress has been made which is described in section 2.3.

The practice of the ECWP is to work closely with the atomic collisions theorists at Auburn University, Alabama, USA and with astrophysics colleagues at the University of Cambridge, UK and with the CLOUDY team at Georgia State University, USA. This is evident in the publications achieved over period 3 and is of quite unambiguous mutual advantage to fusion and astrophysics.

Three meetings took place during period 3 connected to ECWP activities. The first, at the JET Facility 25-27 April 2012 brought together Prof. Badnell (Strathclyde University and ADAS-EU), Prof. Bogdanovitch (Vilnius University), Drs. Quinet and Palmeri (Mons-Hainaut) and the ADAS-EU team based at Culham Laboratory (Prof. Summers, Dr. O'Mullane and Dr. Giunta). It had a dual purpose of a joint meeting between the task force leaders and spectroscopists at the JET Facility and the ECWP specialists to discuss JET needs and to explain the status and implications of the ADAS-EU studies. Secondly, it was an opportunity for the ECWP to examine together the problems of structure code unification and exploitation. The joint meeting was addressed by Dr. O'Mullane who summarised ADAS tungsten modelling and by Drs. Groth and Brezinsek (task force leaders who presented JET interests from the modelling and experimental points of view). The second was the ADAS Workshop at Cadarache 23-29 Sept 2012, which was opportunistic from the ECWP point-of-view. Presentation of DR results was made by Dr. Schippers (Justus-Liebeig University, Giessen). This provoked discussion of the handling of threshold resonances in DR from the collisional-radiative perspective and the combining of fusion and astrophysical ideas - especially with Prof. Ferland (Gerogia State University). This is discussed in section 2.1 here. The third meeting took place at the JET Facility 10-12 Dec 2012, almost at the end of the ADAS-EU project, and brought together Prof. Badnell, Prof. Summers and Dr. Pameri to assess the state of code merging reached and to plan the future after ADAS-EU. This is discussed in section 2.3.

Chapter 2

Review of progress 2012

2.1 Dielectronic recombination developments

Threshold resonance structure in dielectronic recombination for open d and open f subshells

In this period, investigation has continued into the consequences for dielectronic recombination of the threshold resonant structure measured in W^{+20}. The JustusLiebig University group has followed up with similar measurements on adjacent ions W^{+18}, W^{+19} and W^{+21}. Additionally there are the older results on Au^{+25}. We now see the pattern of behaviour progressively through f-shell ions. Theoretically, the explanation lies in very large configuratiuon interaction only a portion of which can reasonably be included in conventional calculation. The statistical ergodic-like behaviour through these autoionising states leads to a dilution of the Auger rates and so enhancment of DR. A solution though which spans all temperature regimes is still being worked on. The current state is given in our publication [1] from which the following information is extracted: "In recent years, there has been significant interest in the dielectronic recombination (DR) of complex ions involving open d and open f subshells. Experimental measurement of DR in Au^{+25} (Hoffknecht et al 1998 J. Phys. B: At. Mol. Opt. Phys. 31 2415) and W^{+20} (Schippers et al 2011 Phys. Rev. A 83 012711), both with ground configurations of $4p^6 4d^{10} 4f^8$, revealed extremely large and broad resonances at low electron energies. DR in such ions is very difficult to describe in detail theoretically because of the complexity of the recombining resonant states and the source of these resonant structures has not been fully explained for the aforementioned ions. However, a very recent measurement of DR in Au20 + (Schippers et al 2011 Phys. Scr. T 144 014039) with a ground configuration of $4p^6 4d^{10} 4f^{13}$ displayed very large but narrower resonances in the low-energy region. With the somewhat reduced complexity of the recombining resonances in this ion, we have been able to complete the first full intermediate-coupling level-resolved DR calculation for Au20 +. In the low-energy region, we find excellent agreement with the experimental measurements, and have been able to show that the DR rate coefficient in this ion is completely dominated by δn = 1 transitions and that the low-energy resonances are primarily due to recombining levels of the $4d^{10} 4f^{12} 5lnl'$ configurations as suggested by Schippers et al (2011 Phys. Scr. T 144 014039) based on atomic structure calculations."

Isoelectronic dielectronic data production for generalised-collisional-radiative emodelling

Work has continued on state-selective dielectronic recombination data production (ADAS formast *adf09*) for isoelectronic sequences in *ic* resolution. The last completed sequence is Al-like [2]. The size of the datasets is now becoming prohibitive and so it is unlikely that the fully resolved calculations will be continued to further sequences. With the move to medium-weight and heavy element ion, the preferred route to the high level DR capture is to use the bundle-nl projection/condensation technique (see Summers *et al* , 2006 [3]), but low level recombined and recombining states require *ic*-resolution. The *bbgp* approximation introduced by Summers (and further developed for ADAS-EU) can fulfill this need, but the conventional AUTOSTRUCTURE post-processing to *adf09* can itself impose the summing over intermediate states. This is called the *hybrid* method. It has been perfected in this period at the same time as incorporating a pure configuration average (*ca*) DR capability in AUTOSTRUCTURE. The *adf09* format and access

routines have been modified to accomodate these changes. Mass production will begin shortly. A trial associated with astrophysical needs has been carried out using many elements by Kasen *et al* 2013 [4].

2.2 Distorted wave *adf04* dataset production for neutral and near-neutral medium-weight elements

The distorted wave cross-section extensionj to AUTOSTRUCTURE has been worked extensively by Summers and Giunta over 2012 to uprate the baseline of ADAS *adf04* datasets to level 1 precision in both *ls* and *ic* resolution. Scripts for automatic distributed processing have been implemented by Prof. Summers. Additionally scripts for web procurement, assembly and integration of standard (NIST) energy levels and assignments into special *adf04* datasets have been implemented. These are refreshed periodically so that the whole system is systematically maintained and updated. The special issue to which attention is drawn here is the improvement of the data for neutral and near neutral medium weight atoms and ions by optimising of the AUTOSTRUCTURE calculations. There are a number of controls available for such improvement including selective orbital imnprovement, improvement by extended configuration interaction and the inclusion of pseudostates. We have sought prescriptive approaches which can be applied semi-automatically to series of neutral and near neutral atoms. Currently this has been done for n=3 shell ions. Additionally, the ability of AUTOSTRUCTURE to use observed energies both at the *ls* and *ic* resolutions in adjustment of the Hamiltonia has been used at the last steps. This provides our completion of the AUTOSTRUCTURE *DW* exploitation for ADAS. Very extensive such data amounting to many giabytes has been added to the ADAS *adf04* libraries and issued.

2.3 Special studies of key tungsten ions foir influx measurement

From the starting point of the *adf04* datasets for W^0 - W^{+5} based on the Mons-Hainaut and Vilnius atomic structures (see sub-contracts S2 and S4), extended into the collisional domain with the plane-wave-Born *PWB* approximation, we have sought in 2012 to take this to a higher level. The plan has been to make AUTOSTRUCTURE structure calculations which match exactly the solutions obtained by the Mons-Hainaut (Cowan) code and the Vilnius code. We have held two special ECWP meetings at the JET Facility in pursuit of this objective (see appendices A.1 and A.2). This work is not complete, but aspects of the strategy are now clear. For the Vilnius match, the numerical radial wave functions can be imported into AUTOSTRUCTURE. An interface between Cowan (in fact and HFR+CPOL code) and AUTOSTRUCTURE is more problematic because of the way the Hamiltonian is built. A number of avenues and exploratory calculations have been made. Although these give quite good correspondences, they fall short of a true like-for-like solution. Prof. Badnell, Dr. Palmeri and Prof. Bogdanovitch will continue in the collaboration initiated in ADAS-EU in pursuit of these objectives.

It is noted that our ADAS colleagues at Auburn University, Alabama have made progres in using large scale R-matrix calculations for low tungsten ions (ballance *et al* , 2013 [5]

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[4] D. Kasen, N. R. Badnell and J. Barnes. 'Opacities and soectra of the r-process ejecta from compact object mergers'. Astrophys. J., **774**(25) (2013) 13

[5] C. P. Ballance, S. D. Loch, M. S. Pindzola and D. C. Griffin. 'Electron-impact excitation and ionisation of W^{+3} for the determination of tungsten influx in a fusion plasma'. J. Phys. B, **46** (2013) 055201

Appendix A

ECWP documents

A.1 ADAS-EU ECWP Meeting EFDA-JET Facility,CCFE Culham Laboratory, Abingdon, UK. 26-27 April 2012.

location: EFDA-JET Facility,CCFE Culham Laboratory, Abingdon, UK.
Date: 26-27 April 2012.
Present: Nigel Badnell, Pascal Quinet, Patrick Palmeri, Pavel Bogdanovitch, Martin O'Mullane, Hugh Summers.
Present (TF session): Mathias Groth, Sebastjan Brezinsek, Kerry Lawson, Andy Meigs, Constanza Maggi, Mike Stamp and others.

Purposes: Progress the electron collision working party activities for ADAS-EU.
Discuss tungsten needs for JET and ECWP/ADAS developments for tungsten.

Items:

1. 26 April and the afternoon of 27 April were devoted to technical discussions on atomic structure and collision cross-sections amongst ECWP members. The morning of 27 April was committed to a colloqium with the ECWP ADAS-EU team, representatives of the JET task forces (MG and SB) and JET/CCFE spectroscopists and spectral analysts.
2. The very large multi-configuration interaction structure codes of Prof. Bogdanovitch are operational and, with the help of Prof. Badnell, include a plane-wave Born pathwath (*PWB*) to production of ADAS *adf04* datasets.
3. With the delivery of the the set of Vilnius *adf04* datasets as specified in sub-contract S3, the ECWP was supportive of a follow-on sub-contract to consolidate and extend the Vilnius *PWB* tungsten calculations.
4. Prof. Summers was concerned about contributions from 5d - 5f transitions in ions such as W^{+2}. Simplified baseline ADAS calculations indicated that such transitions would carry significant radiated power, yet they are excluded from the Mons-Hainaut analysis.
5. Prof. Bogdanovitch indicated that his code was not set up for multi f-shell occupancy and therefore, although he could address 5d-5f promotions, the full configuration action would not be present.
6. It was agreed to include 5d-5f transitions in the Bogdanovich quasi-relativistic (TRO) approach. The configuration interaction would be restricted initially to at most one or two f -electron promotions from closed shells. The possibilities for extending the numbers of equivalent f -shell electron capability will be explored with Prof. G. Gaigalas.

7. Prof. Badnell and Prof. Bogdanovitch engaged in a break-off discussion on the possibilities for transfer of an orthogonal basis of radial wave functions from the Bogdanovich multi- configurational with virtual excitations and TRO codes as inputs for the AUTOSTRUCTURE. This is an important issue, since it would allow the higher quality AUTOSTRUCTURE *DW* cross-section calculations based on Bogdanovitch structure. They decided that there was no ambiguity inthe evaluation of the Hamiltonian with the two codes, so simple transfer of the numerical radial wavefunctions could be done. They agreed to follow this up with further collaboration.

8. Prof. Summers concurred with these recommendations and agreed to prepare the follow-on sub-contract S7 funded in place of the cancelled S7 sub-contract with Groningen. See report SUBC2 for details.

9. The ECWP was very satisfied with the links and structure parameter transfer arrangements between Mons-Hainaut established in sub-contract S2 so that ADAS *adf04 PWB* datasets could be prepared.

10. Prof. Summers and Dr. O'Mullane drew attention to the considerable interest of the fusion community in the consequential W^0 SXB ratios and siad that this would be discussed further ihn the joint session on 27 April.

11. In a break-away session, Prof. Badnell and Dr. Palmeri investigated the possibility of upgrading the HFR+CPOL collision strengths to distorted-wave quality by considering an interface between HFR and AUTOSTRUCTURE. They found that this interface needs a long term effort essentially because the construction of the Hamiltonian matrix elements is very different in these two programs, i.e. HFR builds its Hamiltonian with respect to configuration average energies, while this is not the case with AUTOSTRUCTURE which considers all the core-orbital Slater integrals. Another idea was explored consisting in building AUTOSTRUCTURE models in order to reproduce the high-energy limits of the HFR+CPOL PWB collision strengths. Tests were carried out in W^{+4} and agreements between both sets of high-energy limits reached about 20% validating this idea. Further collaborationj was recommended.

12. In their tests of structure compatibility and Born limits, Prof. Badnell drew attention to the necessity of including higher Born multipoles for collisions than would usually be done in pure structure and radiative transition studies. This explains some modest discrepanvcies in these limits between Vinius, Mons-Haianut and ADAS baseline calculations.

13. In view of the success of atomic data transfer between the Mons group and the ADAS team, this work should continue for other elements of interest for fusion - in principle for all these elements for which atomic structure calculations have already been published by Mons-Haianut.

14. Prof. Summers concurred with these recommendations and agreed to prepare a follow-on sub-contract S6. See report SUBC2 for details.

Joint session on 27 April 2012

Items:

1. Mathias Groth spoke on the tungsten atomic data requirements from the point-of-view of impurity transport modelling. He summarised the usgaes in modelling packages such as the JETTO suite with illustrations. Regions of special importance are the divertor and the vicinity of transport barriers. He sought recombination, ionisation and radiated power coefficients for all tungsten ions.

2. Sebastijan Brezinsek focussed on spectral analysis of tungsten ions, especiallr radiators in the divertor and neutral tungsten line emissions as a measure of influx. He referred to FZ-Jeulich experiments and the set of W0 lines observed by them. He sought higher precision SXBs.

3. Martin O'Mullane described ADAS calculations for tungsten. His viewgraphs are attached as appendix A.3.

4. Dr. Brezinsek wished to bring the new ADAS W^0 SXB ratios into use for the current EFDA-JET conference papers in preparation. This led to discussion about the perceived fdelay in formal data release by the ADAS Project and the point at which ic could be 'certified@. Dr. O'Mullane drew attention to the need for further checks, both between different sources (in this caee Mons-Hainaut and Vilnius) and of the contractions of the full set of configurations used in the Mons-Hainaut structure and that which could reasonably be included in the *adf04* datasets.

5. Dr. O'Mullane stated again the problem of hurried adoption of data, with apparent acceptance of caviats and needs for updates and the very common failure of the user community to update properly in a timely manner.

6. Prof. Summers stressed the the real validation step of influx in a generalised-collisional-radiative picture of measuring spectral observables in each spin system of a stage and in an adjacent sequence of stages - in this case W^0, W^{+1} and W^{+2} . He pointed out that the new ADAS-EU work delivered the necessary theoretical data for all three ions.

HPS
8 May 2012

A.2 ADAS-EU ECWP and Molecular Theme Meeting EFDA-JET Facility,CCFE Culham Laboratory, Abingdon, UK. 10-12 December 2012.

location: EFDA-JET Facility,CCFE Culham Laboratory, Abingdon, UK.
Date: 10-12 December 2012.
Present: Nigel Badnell, Pascal Quinet, Patrick Palmeri, Martin O'Mullane, Alessandra Giunta, Kurt Behringer, Francisco Guzman, Hugh Summers.
Purpose: To check and perfect work to-date and aspects to be followed up after ADAS-EU.

Items:

1. The development of the ADAS-EU H_2 molecular vibronic collisional-radiative model has been a difficult ands complex task. The meeting draws together Dr. Guzman, Dr. O'Mullane and Prof. Summers with Prof. Behringer (an expert in observing H_2 isotopmer molecular spectra in the visible) to critically examine results, identify and correct errors. It is also a last opportunity for a critical overview.

2. The meeting has a second ECWP non-overlapping objective of assessing progress on the Mons-Hainaut (Cowan structure) /Strathclyde (Autostructure) alignment.

3. Separate groups worked on items 1 and 2.

4. Prof. Badnell and Dr. Palmeri consider that they now have a clear understanding of the Cowan handling of closed shells and believe that it is probably compatible with Autostructure.

5. Prof. Badnell and Dr. Palmeri set themselves the task of matching Autostructure to Mons for E1 transition probabilities of W^{+5}. Initial efforts were quite good ($\sim$ 15%) and they decided to move on to an initial assessment also of W^{+4}. One discrepancy noticed was in fine structure.

6. They checked Born limits and noted Mons-Hainaut (up to $\lambda = 2$), Vilnius (up to $\lambda = 3$) and Strathclyde (up to $\lambda = 4$). The latter is required for collisions and leads to better Born limit agreement. It seems that agreement is reached of $\sim$ 10-15% for A-values and Born limits and $\sim$ 2% for energies. This is almost acceptable but is of course not a true cross-aligment.

7. Prof. Badnell and Dr. Palmeri would like to carry on with W^{+3} down to W^0 over the next few months to see what can be achieved in the most difficult cases.

8. A forward work plan is evolving. Dr. Palmeri will work more closely with Autostructure to see if he can use its flexibility to match much more closely with Cowan. Prof. Badnell will will work on the actual breakdown of the Hamiltonian. It may be that root and branch appraisal of Cowan and Autostructure and substantial supplementary coding may be required for precise matching.

9. Prof. Summers pondered if the actual Hamiltonian for the two codes with the same configurations might in a purely alegbraic manipulation give a correction transformation from one code to the other.

10. Prof. Behringer reviewed H_2 ground electron state vibrational substate populations generated by Dr. Guzman's code with expectations from ASDEX and some of the partial results he had from Wundelich. Discrepancies were discovered and code corrections made. It cannot be said yet that there is certainty of an error-free code.

11. Prof. Behringer worked on the fine ro-vibrational spectral identification of the Fulcher bands of D_2 from recent JET spectra. For this he used his own Visual Basic code. The matching was very convincing and Prof. Behringer felt confident in identifying also very weak HD emission.

12. Prof. Summers and Prof. Behringer agreed to work on in 2013 on making an ADAS rovibrational spectral analysis IDL display code which emulated the Visual Basic code.

13. Dr. O'Mullane worked with Dr. Guzman on the final ADAS versions of series 9 codes and accepted criticisms from Prof. Behringer and made changes accordingly.

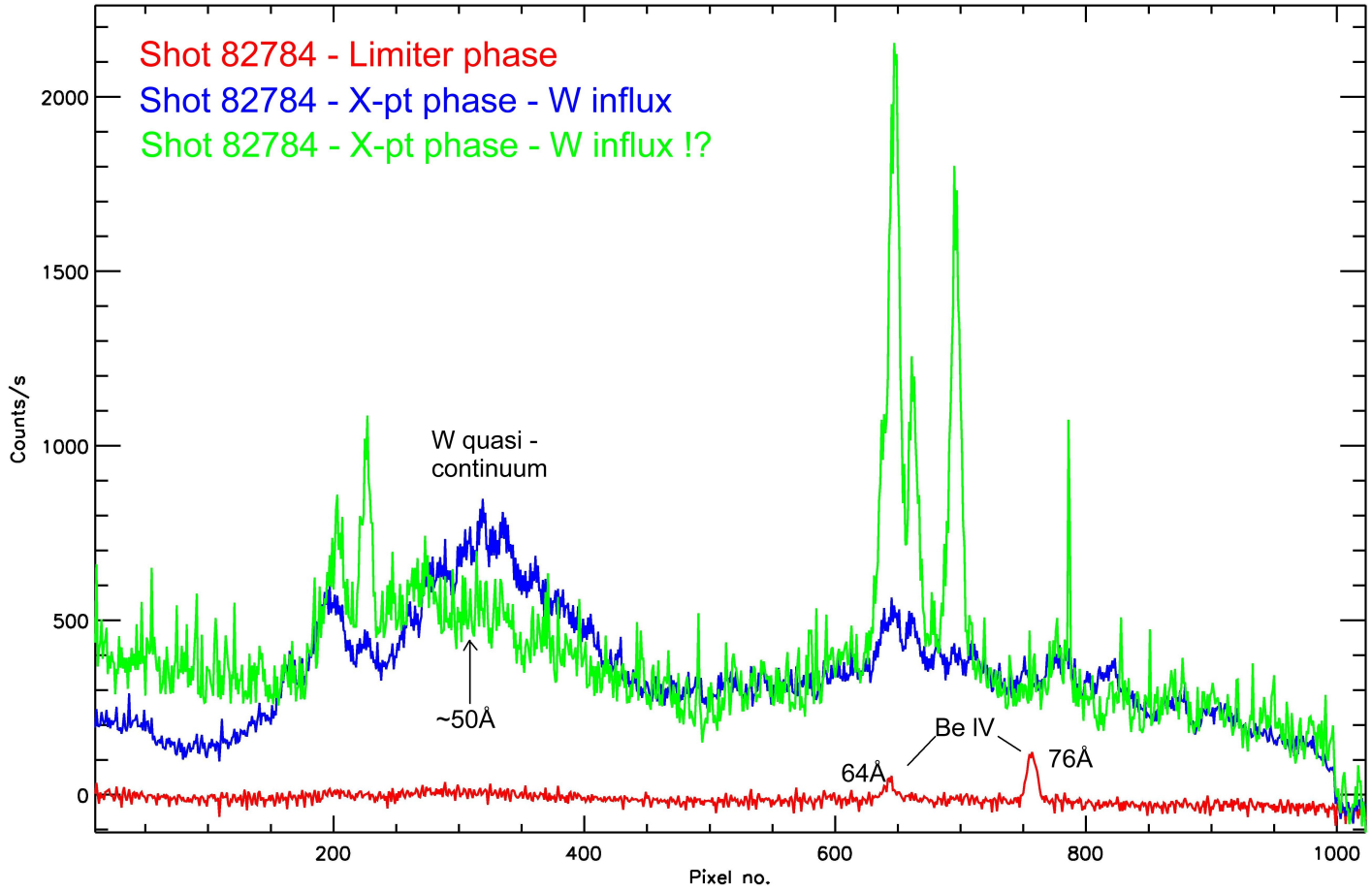
HPS
14 December 2012

A.3 Presentation at joint meeting JET Facility 27 April 2012 by Dr. Martin O'Mullane.

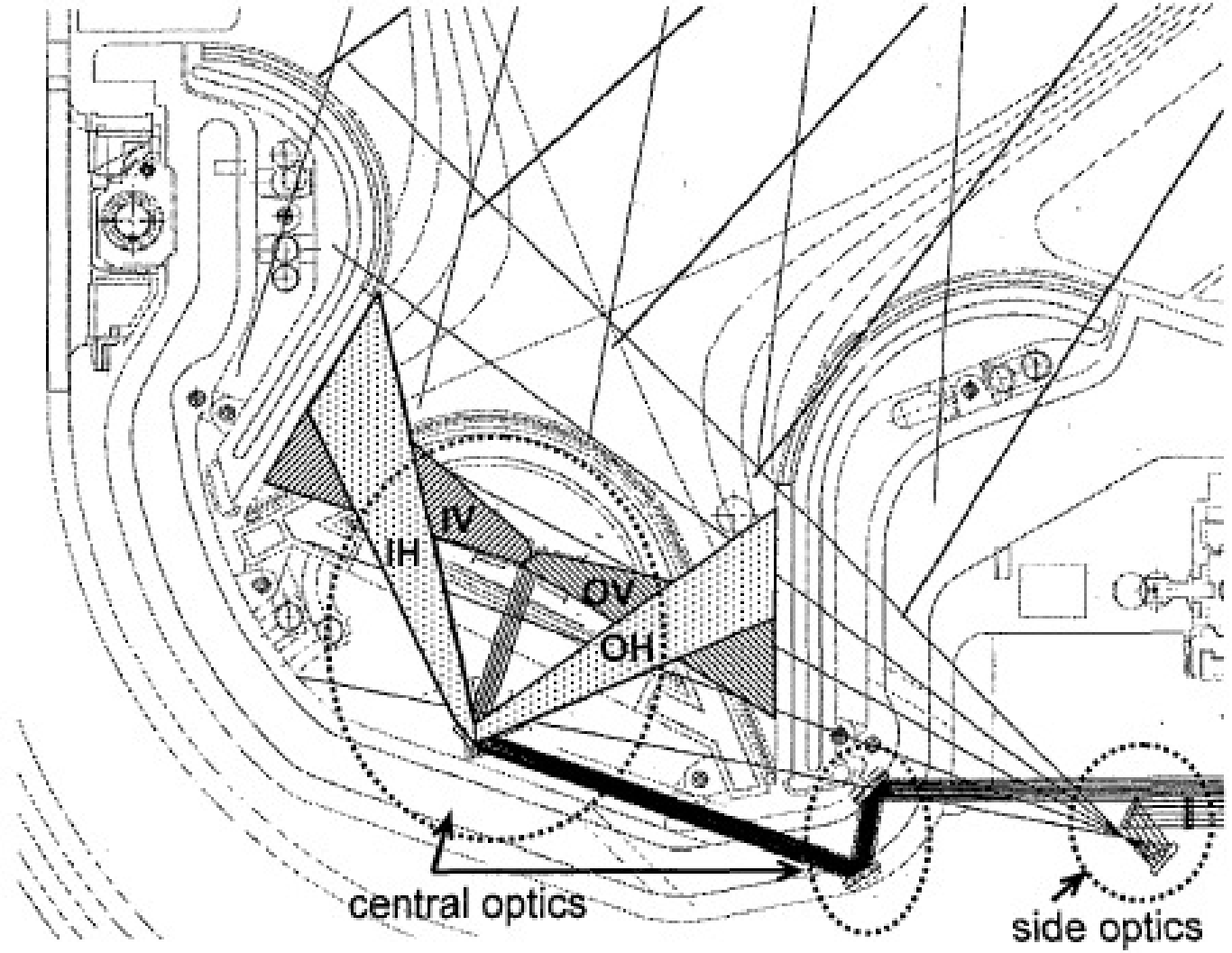
Status of Tungsten data in ADAS

JET's ITER-like wall: ILW

Beryllium plasma facing components with a tungsten divertor.



Proposed divertor spectroscopy for ITER



Areas where atomic data for tungsten is needed

- Neutral and near-neutral species for influx measurements via visible spectgroscopy.
- Strong isolated emission lines in the soft X-ray and VUV from tungsten ion stages with 1–3 optically active electrons arising in the confined plasma.
- Ionisation and recombination coefficients which are density dependent for ionisation (and power) balance calculations.
- Low ionisation stages, $\mathrm{W}^{0} - \mathrm{W}^{+35}$ for divertor and edge modelling.
- Reduction in uncertainity of recombination rates for stages up to W^{+21}.
- Methods to reduce the size and complexity in handling tungsten data.
- Quantification of the influence of active emission from tungsten during neutral beam heating and its contribution to the overall stopping of the beams.

Require *adf04* data for most of these tasks

- Cowan code (`adas8#1`) for baseline production with plane wave Born rates.
- R-matrix sequence data — H, He, Li, F, Ne and Na-like to Kr.
- Other isolated species — all Be, B, some C, O and N.
- `AUTOSTRUCTURE` for complementary baseline — DW accounts for spin changing; input for R-matrix.

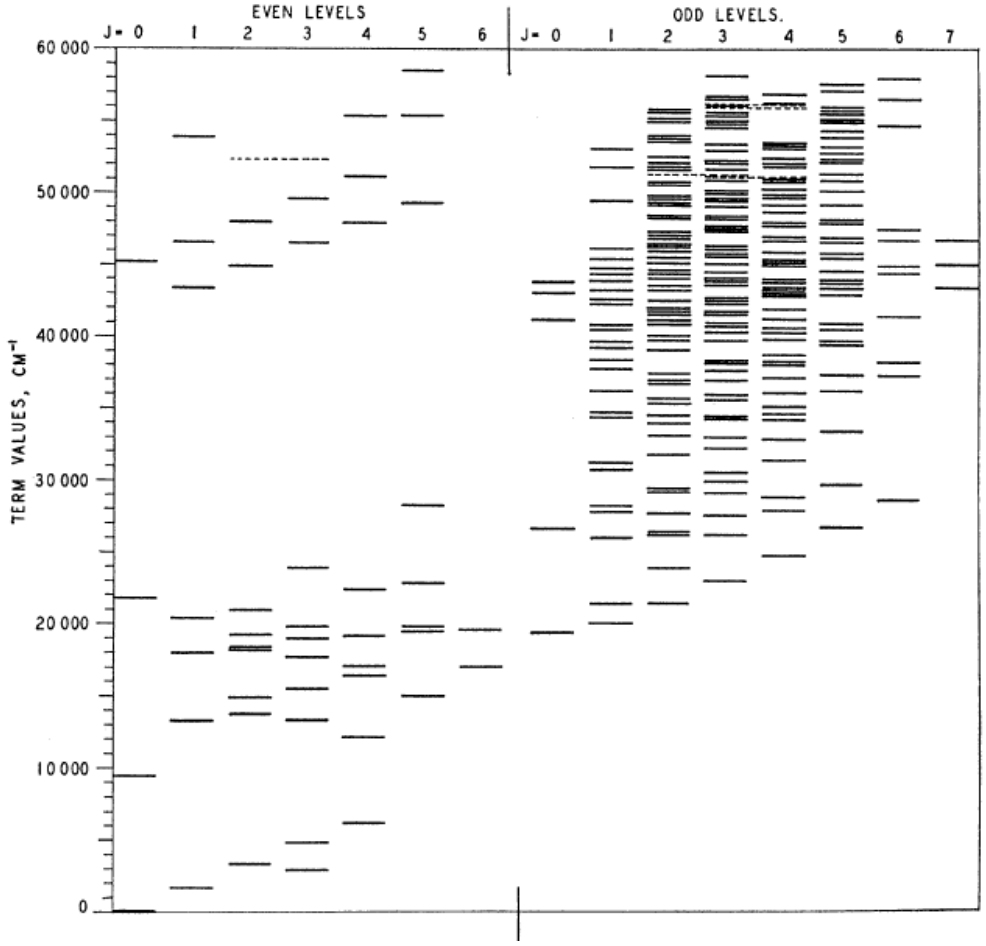
Better structure leads to believable rates

How to improve what we have?

- Mons-Hinaut ASPECT group with improved Cowan.
- Villnius group with massive CI, pure *ab initio* structure.

Harness these efforts as inputs for ADAS collision codes and population modelling. ADAS-EU FP7 has enabled this collaboration.

Consider neutral W



O Laporte and J E Mack, Phys. Rev, 1943

Latest revision: A E Kramida and T Shirai, J Phys Chem Ref Data, 2006

W0 energy levels and our favourite line

			baseline	Mons	NIST
1	4FE 5D4 6S2	(5)2(0.0)	0.0	0.0	0.00
2	4FE 5D4 6S2	(5)2(1.0)	1467.9	1785.2	1670.29
3	4FE 5D5 6S1	(7)0(3.0)	-	2981.7	2951.29
4	4FE 5D4 6S2	(5)2(2.0)	3189.4	3469.8	3325.53
5	4FE 5D4 6S2	(5)2(3.0)	4863.1	4927.4	4830.00
6	4FE 5D4 6S2	(5)2(4.0)	6404.8	6207.7	6219.33
7	4FE 5D4 6S2	(3)1(0.0)	12950.2	9612.9	9528.06
8	4FE 5D4 6S2	(3)5(4.0)	14044.2	12249.8	12161.96
9	4FE 5D4 6S2	(3)1(1.0)	17084.9	13500.8	13307.10
10	4FE 5D4 6S2	(3)4(3.0)	16981.1	13506.3	13348.56

	NIST	U Mons	*adf04*	
E_{ground}	0.00	-88.0	0.0	$5d^4\,6s^2\ ^5D_0$
E_{lower}	2951.29	2893.0	2981.7	$5d^5\,6s\ ^7S_3$
E_{upper}	27889.68	27815.7	27905.5	$5d^4\,6s\,6p\ ^7P_4$
				$5d^5\,6p\ ^7P_4$ (NIST)

W0 — 4009Å and 5224Å identifications

The `adas8#1`/Cowan generated dataset considers the upper level to be $5d^4\,6s\,6p$ with a leading percentage of 67% for ^7P, 22% from other terms in this configuration and 2.62% of $5d^5\,6p\ ^7P$. NIST identifies the upper configuration as $5d^5\,6p\ ^7P$.

Identifications before 1960 and the isotope shift work of Aufmuth (J Phys B, 1988) confirm our classification.

What about the strongest KS8 line?

	NIST	U Mons	*adf04*	
E_{lower}	4830.0	4838	4927.4	$5d^4\,6s^2\ ^5D_3$
E_{upper}	23964.0	23958	24047.8	$5d^4\,6s\,6p\ ^7D_2$

There is no ambiguity in identifying this line but the purity of the upper level, $^7D_2$, is just 44% with 24% due to the the quintet $^5P_2$ indicating that the spin systems are not pure.

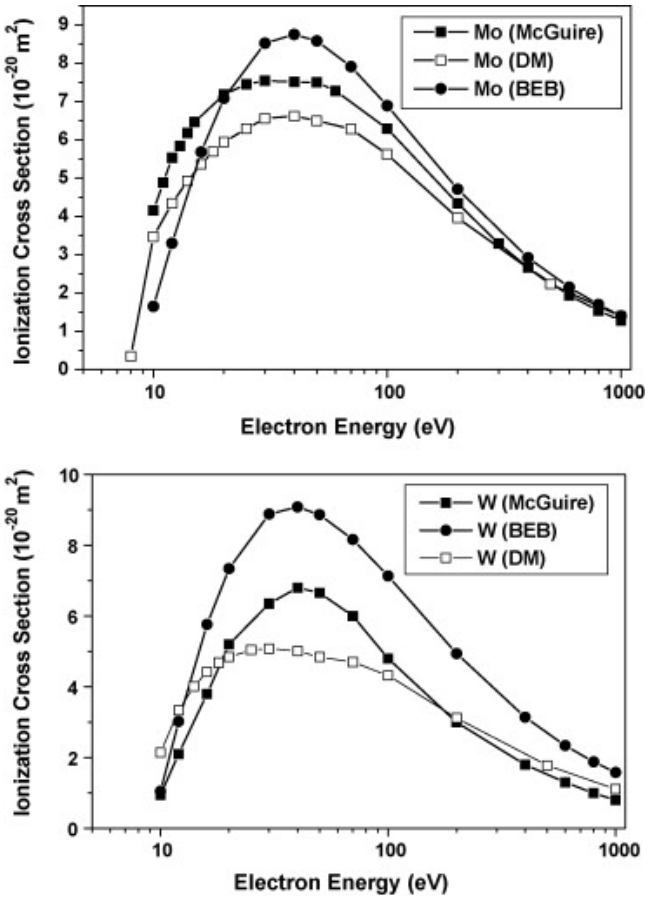
W2+ — emission centered ∼2500Å

			Mons	Villnius	NIST
1	4F14 5S2 5P6 5D4	(5)2(0.0)	0.0	0.00000	0.00
2	4F14 5S2 5P6 5D4	(5)2(1.0)	2291.8	2305.36163	2256.20
3	4F14 5S2 5P6 5D4	(5)2(2.0)	4505.3	4612.69852	4461.19
4	4F14 5S2 5P6 5D4	(5)2(3.0)	6280.7	6506.98415	6277.81
5	4F14 5S2 5P6 5D4	(5)2(4.0)	7615.0	7978.78109	7686.68
6	4F14 5S2 5P6 5D4	(3)1(0.0)	10037.4	10683.80603	9904.30
7	4F14 5S2 5P6 5D3 6S1	(5)3(1.0)	10918.1	12168.55197	10968.54
8	4F14 5S2 5P6 5D3 6S1	(5)3(2.0)	12439.1	13707.06921	12427.09
9	4F14 5S2 5P6 5D4	(3)1(1.0)	12949.8	13735.38143	12881.03
10	4F14 5S2 5P6 5D4	(3)5(4.0)	13803.7	15238.78272	13700.95

Villnius method is just *ab intio*.

Ionisation from neutral W

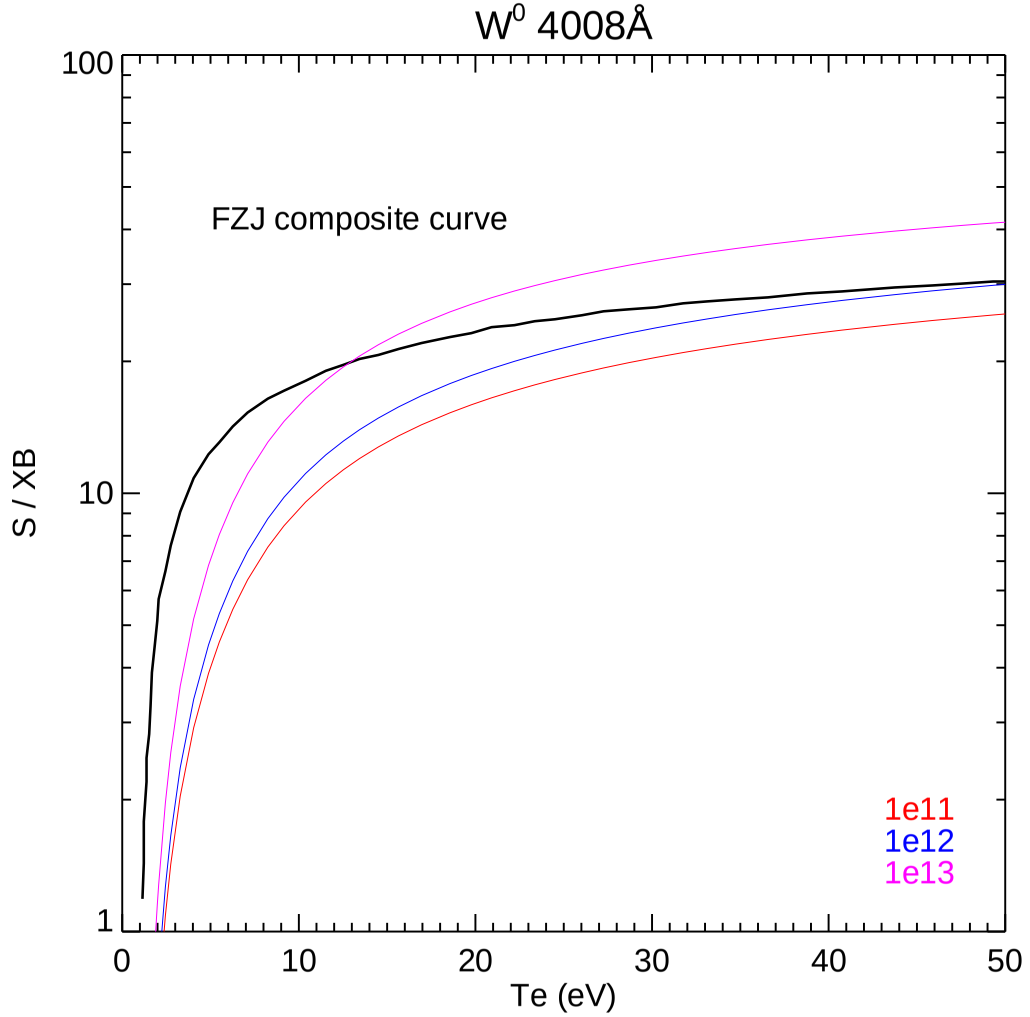
A few to choose from with no great agreement — use range as uncertainty estimate.



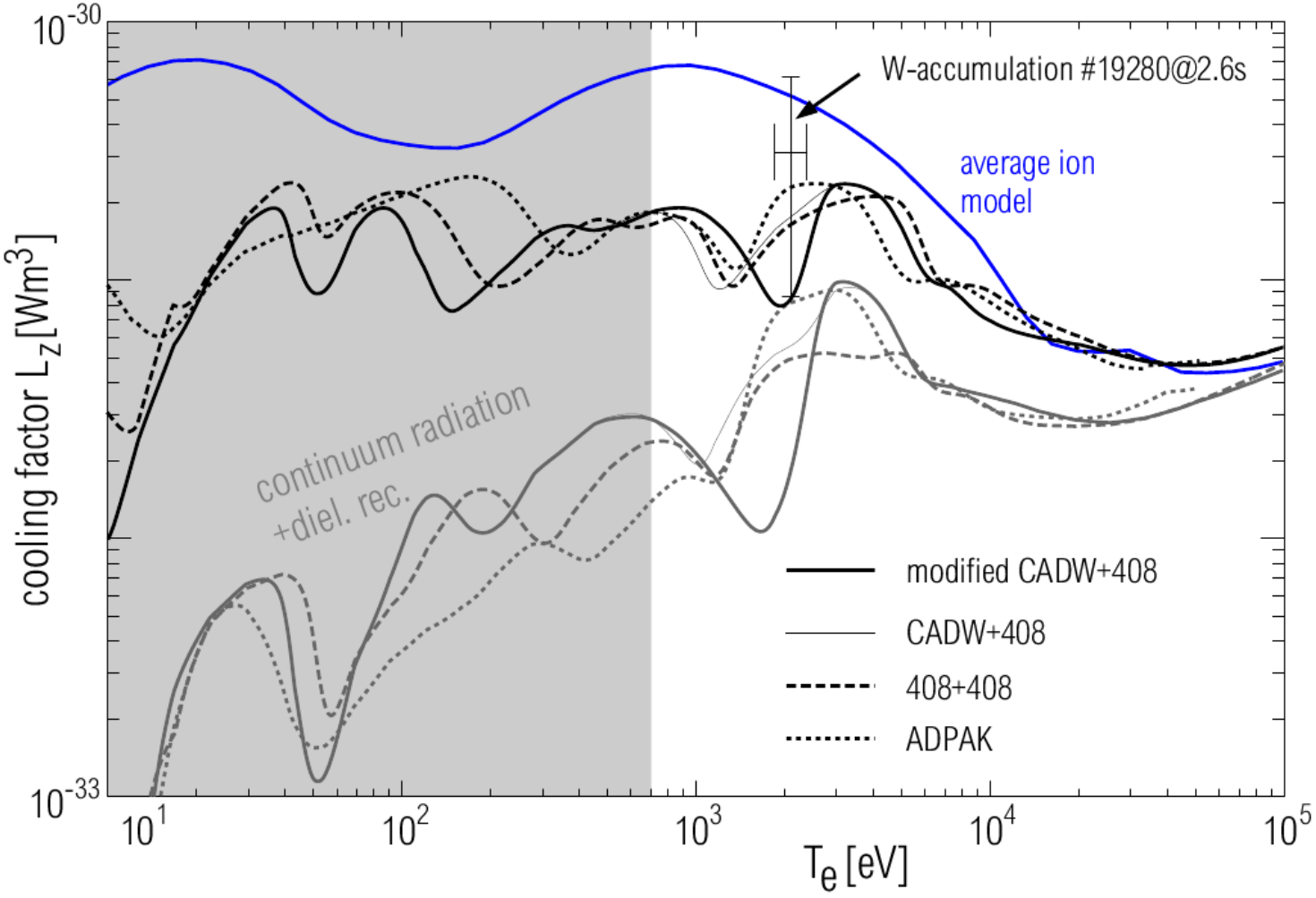
Deutsch et al, Int. J. Mass Spect., 2008

S/XB

If we take Mons *adf04* and CADW *adf07* we get....



Ionisation balance

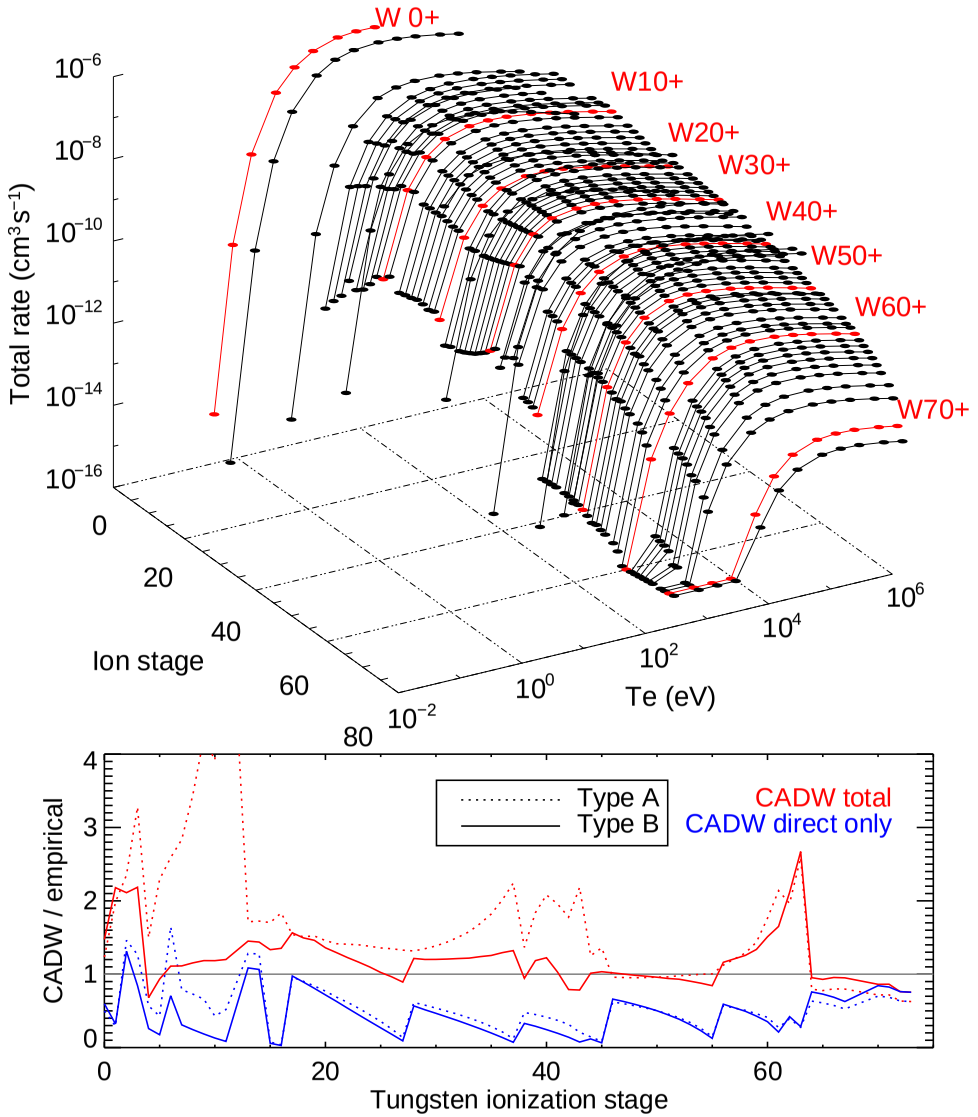


Great uncertainity below 800eV — stages below W^{+28} ($4d^{10}$ ground state).

Ionisation rates

CADW zero-density complete collection — adas8#2.

Loch et al, Phys. Rev. A, 2005



Dielectronic recombination for W^{+20}

Measurement and theory refining rates required for ionisation balance.

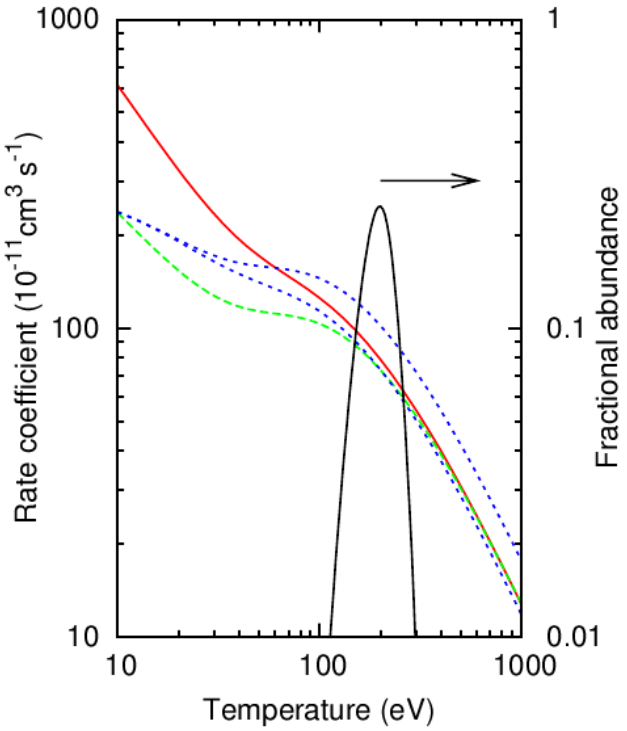


FIG. 7: (Color online) W^{20+} total Maxwellian DR rate coefficients: IC (solid red curve), LS (long-dashed green curve), and CA with-and-without $n = 5$ continuum (short-dashed blue curves). The fractional abundance of W^{20+} in a magnetic fusion plasma is shown also (solid black curve).

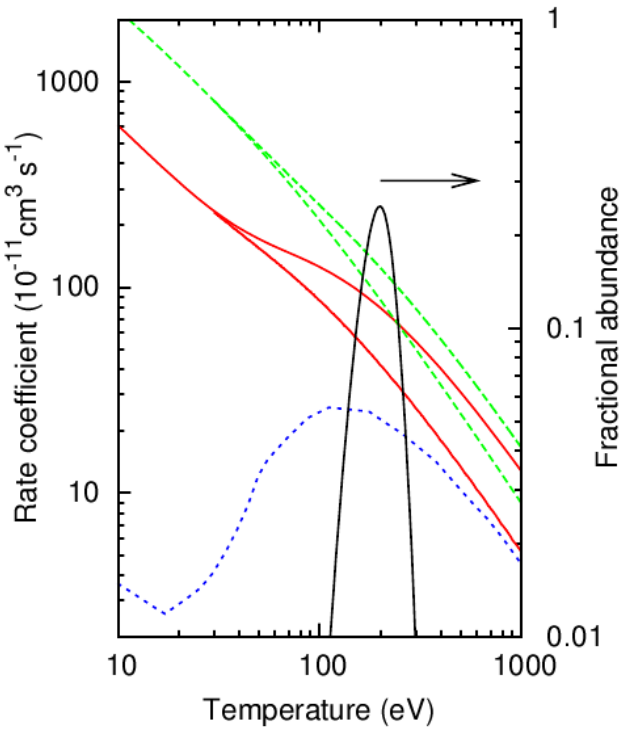


FIG. 8: (Color online) W^{20+} total Maxwellian DR rate coefficients: IC all resonances and to 140 eV only (solid red curves), experiment [7] to 140 eV and with theory top-up for resonances above 140eV (long-dashed green curves), and ADAS [31] (short-dashed blue curve). The fractional abundance of W^{20+} in a magnetic fusion plasma is shown also (solid black curve).

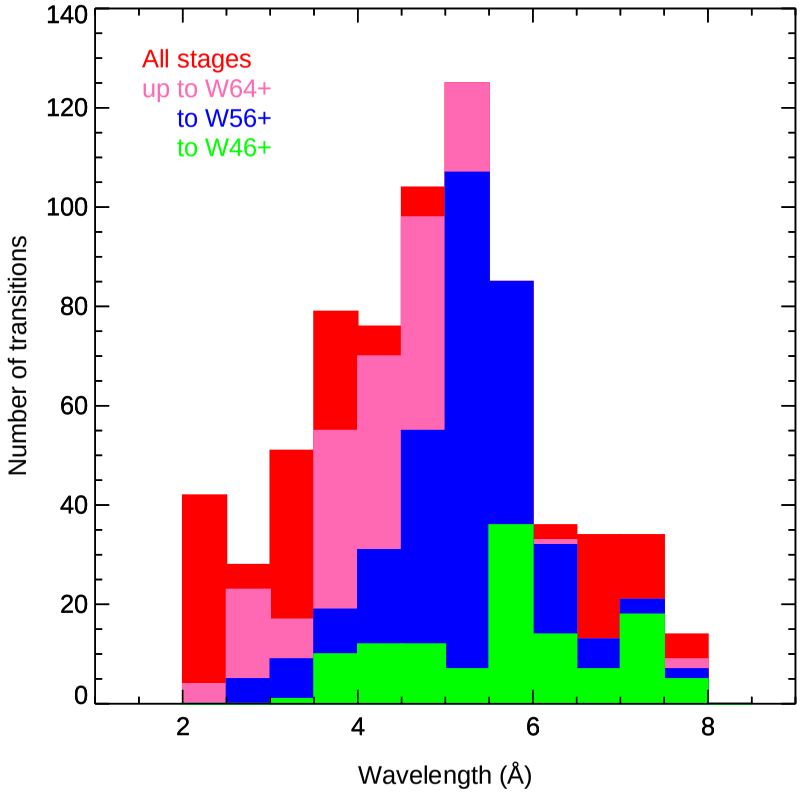
Badnell et al, submitted

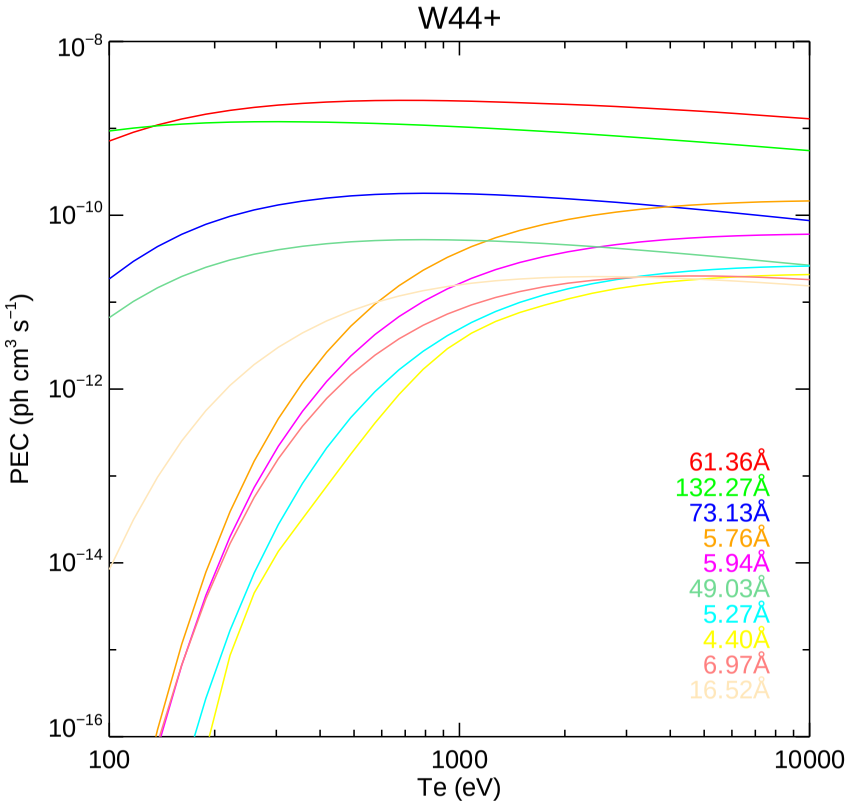
to Phys. Rev. A

Density dependence of S and α

- Not in CADW ionisation or *adf09* DR rates.
- Comes from GCR model.
- Serious revision of empirical formula used to date.
- Plant `adas316` dependence on S and α.

Tungsten emission in the confined plasma





- W38+ to W73+ contribute lines to the 2–8Å spectral region.
- Strongest lines not necessarily in the X-ray spectrum.
- 708 distinct lines.

Relativistic R-matrix calculations

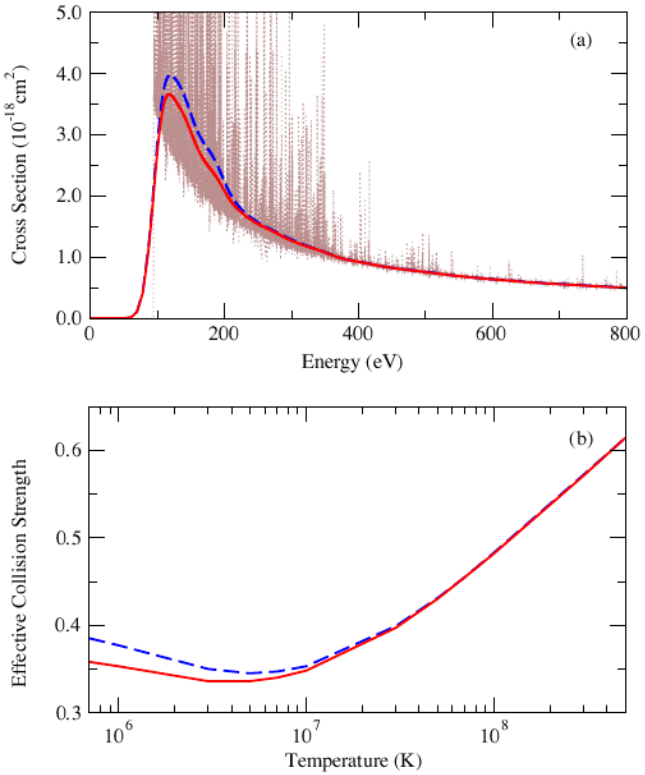


Figure 2. Electron-impact excitation of W^{44+} from the ground state to the $4s4p(1/2, 1/2)_1$ level (level 3). (a) The dotted curve is the damped cross section, the dashed curve is the undamped cross section convoluted with a 30 eV Gaussian, and the solid curve is the damped cross section convoluted with a 30 eV Gaussian. (b) The effective collision strength, where the dashed curve is with no radiation damping and solid curve is with radiation damping.

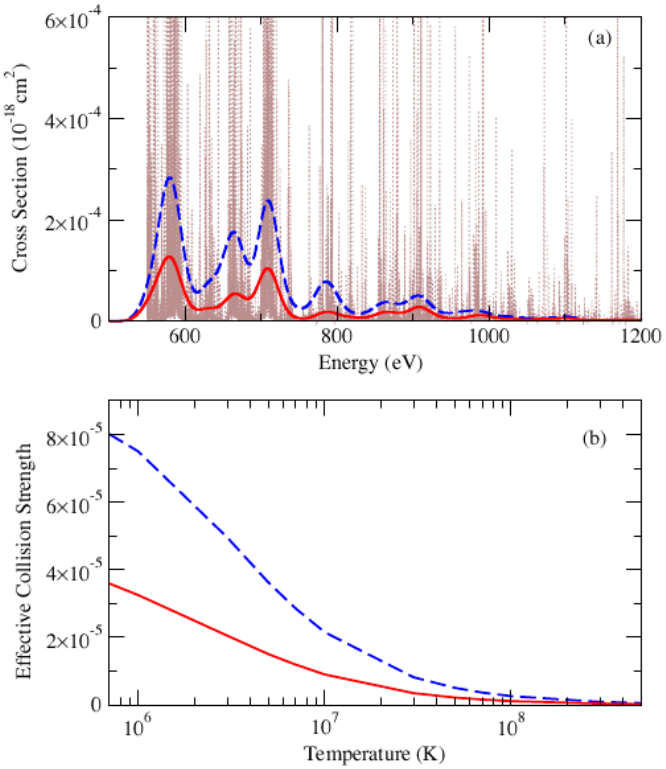


Figure 3. Electron-impact excitation of W^{44+} from the ground state to the $4p4d(3/2, 3/2)_0$ level (level 24). (a) The dotted curve is the damped cross section, the dashed curve is the undamped cross section convoluted with a 30 eV Gaussian, and the solid curve is the damped cross section convoluted with a 30 eV Gaussian. (b) The effective collision strength, where the dashed curve is with no radiation damping and solid curve is with radiation damping.

Apply these techniques to diagnostically significant emitters — Electron Collision Working Party (ECWP) intitiative.