ADAS-EU
ADAS for fusion in Europe

Grant: 224607

Hugh Summers, Martin O'Mullane, Francisco Guzman and Luis Menchero

# ADAS-EU setup report 2

22 June 2010

Workpackages : 22-1-2, 22-2-1, 23-1-2, 23-2-1, 25-1-2, 25-2-2, 26-3-2
Category : PP

# ADAS-EU setup report 2

Hugh Summers, Martin O'Mullane, Francisco Guzman and Luis Menchero

Department of Physics, University of Strathclyde, Glasgow, UK

**Abstract:** *The report reviews setup task completion for project months 10-18*

# Contents

# Preface

This set-up report is the second of a series of three such reports, deliverable under the ADAS-EU project, which summarise the setting-up activities.

**H P Summers**
22 June 2010

# Chapter 1

# Overview

The milestone STP2 concerns 'Training and placement of PDRA2 complete at IPP Garching, report of local on-site support targets available; second sub-contracts (S2, S3) negotiated and active. Decisions on work package extensions' and was scheduled for completion by month 9 and the associated report SETUP2 to be available at month 10. The scheduling of completion and has been moved to month 18 for the reasons summarised below.

PDRA2, Dr. Luis Menchero, is appointed and was in post at 1 Feb. 2010 - a delay of seven months. The training schedule was adjusted to accomodate this. Following this placement and the implementation of sub-contracts S2, S4, S5, S8 in milestone STP1, sub-contracts S3 and S6 have been put in place as part of STP2. Implementation of S7 is inappropriate until PDRA1 is on location at CEA Cadarache. Sub-contract S1 has been designed but not yet implemented - see section 2.4. Thus S1 and S7 are now part of milestone STP3 and report SETUP3. Planned training of Dr. Menchero has been partly achieved at this tyime. A further portions will take place in July 2010 and October 2010. The final third of his initial training will complete with further local orientation at IPP Garching in Autumn 2010.

Engagement with the scientific programme at IPP Garching will follow a number of directions. The initial list was established in the induction visit by D. Martin O'Mullane ( see section 2.2). It is clear that the scientific links between IPP Garching and ADAS are already strong and the main issue is enabling Dr. Luis Menchero to get up to speed as the on-site link person. It is noted that Professor Kurt Behringer, a member of the ADAS-EU Governance Committee and a former AUG Director at IPP, who is based at IPP Garching will assist as a local mentor for Dr. Luis Menchero. Prof. Behringer has great knowledge of ADAS and its targetting on fusion plasma spectroscopy and modelling from his group leadership days at JET. A push on the lower ionisation stages (<30) of tungsten for 2-D plasma models is the priority along with supplementary thermal charge transfer data to singly ionised species. Then the ADAS inputs to TRANSP, an issue driven from IPP Garching, has to continue and be tightened. On the light elements, nitrogen is now an important species for divertor cooling and update of the ADAS database for nitrogen is sought. On CXS, excited donors H($n > 2$) are of interest with a wish for a universal baseline delivery. This also needs ADAS extended bundle-n model links. All these items are engrossed in the ADAS-EU plans and so rapid progress is expected once the initial settle down and induction period is over.

In summary STP2 has been almost fully met and part of milestone STP3 within this eighteen month timeframe.

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# Chapter 2

# Work package reports

## 2.1 Work package 25-1-2

Preparation of the the ADAS-EU Research Fellow position description (PDRA2) was completed and reissued for advertisement on 21 Oct. 2009. This was approximately three months after the first attempt and was considered an appropriate delay. To increase visibility of the advertisement, it was placed with Physics World in addition to the circulation lists and mechanisms used on the previous occasion. The post descriptor is attached in Appendix A [1] and the Physics World advertisement in Appendix A [2].

The interviews were scheduled for 1-2 Dec. 2009 at Culham Science Centre.

Candidates were short listed by Professor Hugh Summers and Dr. Martin O'Mullane. Applicant details, together with references were circulated to the ADAS-EU Governance Committee members for comment and ranking.

The interview board comprised Professor Hugh Summers (Chair) ADAS-EU Director, Physics, University of Strathclyde; Dr. William Morris, Head of Experiments, UKAEA Culham Laboratory, Professor Kurt Behringer, Retired AUG Director Max-Planck-Institut fuer Plasmphysik, Garching-bei-Muenchen, Germany and Dr. Martin O'Mullane, Physics, University of Strathclyde.

Four candidates were short listed and references taken up. One person withdrew his candidature before interview. One candidate was late in submitting his curriculuum vitae. This was accepted as a communication problem with India and this candidate was instated as a fourth person on the short list. It was possible to interview two candidates in person. Two candidates, located in Argentina and India, were interviewed by teleconference link. One candidate was deemed appointable.

Position PDRA2 (placement Max-Planck-Institut fuer Plasmaphysik, Garching-bei-Muenchen, Germany) was offered to Dr. Luis Menchero and was accepted. The agreed starting date was 1 Feb. 2010. The appointment was therefore seven months later than scheduled.

Interview assesment forms, supplementary interview assessment forms and interview decision forms are archived at Human Resources, University of Strathclyde.

## 2.2 Work package 23-1-2 and 22-1-2

In the view of the final successful appointment of PDRA2 at this stage, but its delayed start, induction training scheduling was adjusted. It is noted that Dr. Menchero is an ion-atom collision theorist with substantial computational experience. He is inexperienced in atomic population and ionisation state modelling for the plasma environment and in general plasma physics. Dr. Martin O'Mullane visited IPP Garching from 3-12 Feb. 2010 for first discussions with Dr. Menchero and with scientific staff at IPP Garching. The report is attached in appendix B [1]. Dr. Menchero visited

JET from 1-12 Mar. 2010 for ADAS orientation and discussions of scientific background and review of progress and intent with respect to ADAS-EU themes and work packages (see Appendix B [2]). It was decided that Dr. Menchero would attend the 17th Culham Plasma Physics Summer Schoool 12-23 Jul. 2010 to fill in background on plasma physics. In view of the proximity of the next ADAS-EU Course, it is decided that Dr. Mechero will attend the course as a participant. It will be appropriate to have a further visit on-site at IPP Garching by Dr. O'Mullane, his ADAS-EU scientific mentor, for one or two weeks in Autumn. This will complete his induction and background training amounting to nine weeks of close engagement with ADAS-EU training staff. This is the originally planned amount. An ADAS-enabled laptop has been procured for the use of Dr. Menchero.

## 2.3 Work package 22-2-1 and 23-2-1

The work package tasks concern annual update training for the PDRAs at UKAEA Culham Laboratory/JET and an on-site visit at point of placement annually by the ADAS-EU mentor. In the light of the delayed appointment of PDRA2, this applies only to Dr. Guzman at this stage. The update training and task evaluation took place from 1-12 Mar. 2010, coinciding in time with the induction training of Dr. Menchero (see Appendix B [2]). At this time Dr. Guzman made a presentation of his molecular development work at Fz Juelich. This is attached as Appendix B [3]. Professor Hugh Summers visited Fz Juelich on 8-9 Jun. 2010 to appraise effectiveness and direction of the ADAS-EU work of Dr. Guzman. The report is attached in Appendix B [4].

## 2.4 Work package 25-2-2: Sub-contract technical specification

### 2.4.1 Atomic data and models for neutral beam diagnostics

For sub-contract work package WP-S6 ("Lithium beam support database update"), a potential European single source was identified which could provide the ADAS-EU requirements. This was the Institute of Applied Physics, Technische Universitaet Wien, Vienna, Austria led by Professor Friedrich Aumayr. A preliminary visit was made by Professor Hugh Summers on 24 Feb. 2010 to assess the capabilities of the group and engage in discussions as to whether and how the objectives could be achieved. The report of the visit is attached in Appendix C [1.1]. It formed the basis for the setting up of the scientific specification for the sub-contract which is attached in Appendix C [1.2]. The sub-contract was specified to have a duration of 12 months.

### 2.4.2 Atomic structure and ionisation for heavy element ions

For sub-contract work package WP-S3 ("Heavy element ionisation cross-sections"), a potential European single source was identified which could provide the ADAS-EU requirements. This was the Department of the Theory of the Atom, Institute for Theoretical Physics and Astrophysics, University of Vilnius, Vilnius, Lithuania led by Professor Alicija Kupliauskiene. A preliminary visit was made by Professor Hugh Summers on 31 Mar. - 1 Apr. 2010 to assess the capabilities of the group and engage in discussions as to whether and how the objectives could be achieved. The report of the visit is attached in Appendix C [2.1]. It formed the basis for the setting up of the scientific specification for the sub-contract which is attached in Appendix C [2.2]. The sub-contract was specified to have a duration of 12 months.

### 2.4.3 R-matrix cross-sections for low ionisation stages of complex atoms and ions

For sub-contract work package WP-S1 ("RMATRIX-II and DARC cross-sections") a European single source was identified which could provide the ADAS-EU requirements. This was the Centre for Theoretical Atomic, Molecular and Optical Physics , Queen's University, Belfast led by Professor Alan Hibbert. A preliminary visit was made by Professor Hugh Summers on 25 Mar. 2010 to assess the capabilities of the group and engage in discussions as to whether and how the objectives could be achieved. The report of the visit is attached in Appendix C [3.1]. The scientific specification for the sub-contract is being set up at this time. This sub-contract has important implications

for coordinated action on electron impact collision data and the exploitation of supercomputer resources in their procurement. Discussions and meetings are taking place on this matter. It is expected that the sub-contract will be put in place within two months. Details will be given in the report SETUP3 in due course.

## 2.5 Work package 26-3-2

The work package task comprises the preparation of this report

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# Appendix A

# ADAS-EU postdoctoral fellowship advertisement

[1] adas-EU_pdra2_post_reissue_HR_details
[2] adas-EU_physics_world_advert_pdra2

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**Ref: JA/R66/2009**

**Principal: Professor Jim McDonald**

# Research Fellow
# (Fixed term to 31 December 2012)
# Circa 30,000 – 45,000 Euros

## Department of Physics

**1. NATURE OF APPOINTMENT**

You will participate in a Euratom Framework 7 Support Action on atomic physics for magnetic confinement fusion research in Europe, called ADAS-EU. You will bring to bear special expertise in atomic data, atomic models, spectroscopic diagnostic methods and the plasma environment at Associated Laboratories of the European Fusion Programme and at the up-coming international fusion project ITER.

You will join a team of experts, linked to the ADAS Project, who have for many years engaged in furthering world fusion research and in sustaining forefront atomic physics inputs to it.

This is an exciting and challenging post for an ambitious and dedicated candidate committed to European collaboration and long-term fusion objectives.

You will be based at IPP-Garching, Germany and will also be responsible for travelling to, and supporting, a number of other European labs. The scientific focus will be on beam related issues (emission, attenuation, charge exchange) as well as the atomic physics aspects of the transport and emission characteristics of tungsten.

More information about ADAS-EU and ADAS may be found at http://www.adas-fusion.eu/ and at http://www.adas.ac.uk.

**Formal interviews for the post will be held on 1st and 2nd December 2009.**

**2. APPLICATION PROCEDURE**

- A letter of application telling us why you have the energy, skills, knowledge and understanding of Higher Education or other 'Not for profit' sectors to make a real difference in the post described.
- A completed application form to which a full curriculum vitae should be attached. The names and addresses of three referees should be given on the application form. The referees may be contacted by the University without further permission from the candidate unless you indicate to the contrary.

Applications should be lodged with Human Resources, University of Strathclyde, McCance Building, 16 Richmond Street, Glasgow, G1 1XQ by **6 November 2009.**

Applicants who wish an acknowledgement of their paper application should address and stamp the enclosed postcard. Online applications will be acknowledged electronically.

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The University operates a normal retirement age of 65 or the September following 65th birthday. Applications will only be accepted from people up to the age of 64 years and 6 months at the date of their application unless otherwise stated. This is in line with the Employment Equality (Age) Regulations 2006.

## 3. ADAS AND ADAS-EU

The Atomic Data and Analysis Structure, ADAS, evolved from an initial structure created at the JET Joint Undertaking in the period 1984-1993. The first objective of the Project, namely the creation of a common software and data package under UNIX was achieved between 1994 and 1996 with the enthusiastic support and funding of leading European fusion and astrophysical laboratories and the agreement and active participation of JET. ADAS has been in a continuing maintenance and extended development phase from 1996 to the present and the Project has expanded to include most of the leading fusion laboratories in the world. The Project is managed by the Department of Physics, University of Strathclyde under the guidance of a Steering Committee.

ADAS for Fusion in Europe, hereafter called ADAS-EU,I s a Framework 7 CSA support activity of four years duration (2009-2012) for efficient implementation of atomic data in plasma diagnostics and plasma modelling at fusion laboratories throughout Europe, for promotion of validation experiments, for management of extended databases of relevant fundamental and applied data and for promotion of key fundamental atomic data calculation and measurement in European Institutions. It will enable improved effectiveness and completeness of analysis of existing fusion experiments and lay all necessary groundwork for ITER and beyond.

## 4. JOB DESCRIPTION

You will play a key role in delivering the primary scientific objectives of ADAS-EU, that is, the provision of analysis tools and necessary atomic and molecular data for atomic and molecular spectroscopy and broadband radiation detection at all wavelengths and in all plasma regions and for plasma models. All these aspects to be in the context of European-wide unified/shared methodologies, databases and maintenance.

There are five main themes: (1) heavy element spectroscopy and models; (2) charge exchange spectroscopy; (3) beam emission spectroscopy; (4) special features; (5) diatomic spectra and collisional-radiative models. You will acquire the ability to support all these areas. You will share leadership in the development of themes 1, 2, 3 and 5. You will be based at the Max-Planck Institut fur Plasmaphysik Garching-bei-München in Germany.

You will receive special training at EFDA-JET in the United Kingdom on ADAS and relating atomic physics to fusion experiments and studies and then you will have the on-site support of an ADAS-EU manager in integrating your activities with the local fusion activities at your placement. In later years you will participate as a tutor in the annual ADAS-EU course for fusion research scientists. You will share in the ADAS-EU series of visits and support to other Associated Laboratories of the European fusion programme.

## 5. PERSON SPECIFICATION

The following criteria are considered essential:-

- PhD in physics, theoretical physics or theoretical chemistry in one of the areas - radiating properties of plasmas, plasma modelling, diagnostic spectroscopic analysis of plasmas, calculation or measurement of electron-ion or atom-ion collisions
- Ability and confidence to use computational tools in support of objectives
- Ability to organise, plan and use time efficiently
- Ability to analyse and then think creatively
- Excellent written and verbal communication skills
- Strong interpersonal skills, friendly and outgoing
- Willingness to keep learning and adapting
- Team orientated
- Willingness to travel

- Preparedness to participate in training – self and others
- Required to publish scientific papers and present at conferences.

The following criteria are considered desirable:-

- Experience of working and collaborating in a large experimental environment - magnetic or inertial confinement devices, astrophysical spacecraft or similar.
- Experience of the computational and data flow infrastructure of large scale experiments.
- Relating to the full scope of a problem - fundamental to applied, theoretical to experimental
- Ability to engage with theorists and experimentalists

## 6. THE DEPARTMENT OF PHYSICS

For further information on the Department, see http://www.phys.strath.ac.uk/.

## 7. THE UNIVERSITY OF STRATHCLYDE

The University of Strathclyde, in the heart of Glasgow, is a vibrant, international, academic community of 16,000 full-time students from 100 countries, and over 3,000 full-time equivalent staff. With a turnover of £220m, we are the third-largest University in Scotland. While still honouring the 200 year old founding vision of Professor John Anderson to be a "place of useful learning", today's Strathclyde is a modern, outward-looking, research-led University with a distinctive reputation for innovation and enterprise. Known for our high entry standards, the quality of our student learning experience, our impressive record on graduate employability and business spin outs, we have led the UK trend by continuing to increase our undergraduate numbers in Science and Engineering.

Within the past two years we have embarked on an ambitious change programme - the Agenda for Excellence - further enhancing the quality of our Research, Education and Knowledge Exchange. This commitment to excellence is supported by major investment in high calibre staff and an ambitious £250m sustainable estate development programme. Already this strategic focus is bearing fruit. Last year we achieved consistent improvement in overall institutional rankings in all major league tables of up to 10 places. According to Research Fortnight, Strathclyde is the only University in the UK top 20 grant earners showing increases in awards in 2006/2007 from all 6 research councils. The Financial Times ranked our Business School's MBA 30th best in the world and first anywhere for value for money.

Presently the University is located on two campuses, the John Anderson (Glasgow City Centre) and Jordanhill (Glasgow West). We are also organised into six main budget areas; our five Faculties (Science, Engineering, Business, Law, Arts and Social Sciences, and Education) and Central Administrative Services, although these structures are also being reviewed as part of our Agenda for Excellence.

## 8. THE CITY OF GLASGOW

Glasgow is the industrial and commercial capital of Scotland and the various groups that have contributed to its population over the centuries have given it a cosmopolitan feel. It has a lively cultural life as home of the national orchestra, opera and ballet and several theatre companies and it possesses a number of fine art galleries; it is the headquarters of the national press and broadcasting media. Its numerous higher and further education establishments have made it a major educational centre.

The Scottish countryside and its splendid recreation and sporting facilities are easily reached from Glasgow.

## 9. SALARY, CONDITIONS OF SERVICE AND BENEFITS

This appointment to the end of 2012 will be made in terms of the enclosed conditions of service, with the exception of the hours of work and annual leave entitlement which will relate to those of equivalent status staff at the laboratory at which the post is based. The appointment will be at Research and Associated Staff grade 7 (current salary in the range €30,000- €45,000 per annum). Salary will be paid in Euros. Annual and/or merit increments will be adjusted to compensate for Sterling/Euro currency movements. Appointees will be subject to the taxation regime of their country of placement.

We also offer staff a range of other outstanding benefits, including:

- Membership of a Final Salary Pension Scheme.
- Training and Development opportunities underpinned by a 10 year commitment to the Investors in People Standard.
- Reduced or remitted fees for vocational and non-vocational study.
- Sports, Recreation and Wellbeing facilities, including Ross Priory, a stunning 17th century house situated in 200 acres of land on the south shore of Loch Lomond, just 40 minutes drive from Glasgow.
- Childcare facilities and voucher scheme.

## 10. POSITIVE ABOUT DISABLED PEOPLE

The University is accredited as a "Positive about Disabled People" employer and operates a guaranteed interview scheme for disabled candidates who meet all of the essential criteria for the post that they are applying for. On the appropriate section of the application form please indicate if you consider yourself to have a disability **and** wish to be considered under the scheme.

The Disability Discrimination Act 1995 defines disability as "a physical or mental impairment which has a substantial and long term adverse effect on a person's ability to carry out normal day to day activities".

Please note that if you indicate that you have a disability then you may be asked to provide information on this at interview. The University needs this information to consider the likely impact of your disability on the duties of the position you are applying for and what reasonable adjustments can be made to the position. This allows the University to comply with the Disability Discrimination Act (1995).

**We value diversity and welcome applications from all sections of the community.**

**The University of Strathclyde is a Registered Scottish Charity, No SCO15263**

LB/ajb
October 2009

**Appendix 1**

## SALARY SCALES FOR RESEARCH STAFF

| Grade | 1 May 2008 | 1 October 2008 |
|---|---|---|
| Grade 6 | £23,692 | £24,877 |
| | £24,403 | £25,623 |
| | £25,135 | £26,391 |
| | £25,888 | £27,183 |
| | £26,665 | £27,999 |
| | £27,466* | £28,839* |
| | £28,290* | £29,704* |
| | £29,138* | £30,594* |
| Grade 7 | £27,466 | £28,839 |
| | £28,290 | £29,704 |
| | £29,138 | £30,594 |
| | £30,013 | £31,513 |
| | £30,912 | £32,458 |
| | £31,840 | £33,432 |
| | £32,795 | £34,435 |
| | £33,780 | £35,469 |
| | £34,793* | £36,532* |
| | £35,858* | £37,651* |
| | £36,912* | £38,757* |
| Grade 8 | £34,793 | £36,532 |
| | £35,858 | £37,651 |
| | £36,912 | £38,757 |
| | £38,019 | £39,920 |
| | £39,160 | £41,118 |
| | £40,334 | £42,351 |
| | £41,545 | £43,622 |
| | £42,791 | £44,930 |
| | £44,074* | £46,278* |
| | £45,397* | £47,666* |
| | £46,759* | £49,096* |
| Grade 9 | £44,074 | £46,278 |
| | £45,397 | £47,666 |
| | £46,759 | £49,096 |
| | £48,161 | £50,569 |
| | £49,606 | £52,086 |
| | £51,095* | £53,650* |
| | £52,628* | £55,259* |

Note: * Contribution Points

***October 2008***


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**Appendix 2**

**CONDITIONS OF EMPLOYMENT**
**RESEARCH STAFF**

## 1. GENERAL CONDITIONS

Members of staff are subject to the Charter and Statutes and the Ordinances and Regulations of the University, published in the Calendar, and to any amendments or additions thereto approved by the University Court and, in the case of the Charter and Statutes, Privy Council.

The University Court recognises the Strathclyde University and Colleges Union (SUCU) as the sole body with which it will negotiate and consult on all collective issues concerned with the terms and conditions of employment of Research staff. Such terms and conditions may be varied by the University Court after negotiation and consultation with SUCU.

Further information on the terms and conditions specified in this document is contained in the Staff Handbook, which also includes further details of such conditions as provision for sick/injury leave and pay, leave of absence, holidays and holiday pay, individual grievance procedures, review and disciplinary procedures and collective agreements. Should you not receive a copy of the handbook on appointment a reference copy is accessible by visiting Human Resources.

## 2. CONTINUOUS SERVICE

In the case of new appointments, unless otherwise stated in the letter of appointment, the date of continuous employment for the purposes of statutory employment rights will be taken to be the date of appointment contained therein. In the case of promotions, regradings or transfers, previous service is continuous.

## 3. ALLOCATION OF POST

The post to which each member of staff is appointed is allocated to the department or other area named in member's letter of appointment and any accompanying papers. Should the University Court deem it necessary, in the furtherance of the objectives of the University specified in its Charter, it shall, having consulted with the parties concerned and having received the advice of the Senate, re-allocate the post and/or the duties pertaining partially or wholly to it to another department or area. Any such re-allocation will be without prejudice to the other conditions of employment of the holder.

If the need arises during the course of employment for members of staff to work outside the U.K. for a period (or periods) of more than one month then such arrangements will be subject to mutual agreement. Members of staff would then be provided with a statement in advance setting out the terms covering such periods of employment.

## 4. RESPONSIBILITY AND SERVICE

Each member of staff is responsible for the proper performance of allocated duties to the person or persons specified in the member's letter and any accompanying papers. Unless otherwise indicated members of staff are appointed for full time service. Members of staff may not accept outside paid employment, including personal consultancies without the permission of Court, which will not be unreasonably withheld.

## 5. WORKING TIME

Working time is that required to fulfil the duties of the post. The University Court recognises that research Staff carry out these duties in a variety of ways appropriate to the nature of the research activity, but expects regular contact to take place between the research staff employee and the supervisor/grantholder (where these positions are occupied by different individuals) during normal working hours on week days. There are exceptions to this pattern which may involve contact at other locations or in the evenings, or at weekends, but these arrangements will be made with the agreement of the member of staff concerned.

Duties may, by arrangement with Head of Department, include some teaching associated with the post (up to a maximum of 40 hours per semester) for which no additional payment will be made.

Additional work which does not fall within the scope of that described above may by arrangement attract payment which must be authorised and processed through the payroll.

## 6. HOLIDAYS

Research staff have an entitlement to accrue days of paid annual holiday at the rate of 2.5 days per calendar month; this equates, for staff employed throughout the leave year, to an annual leave entitlement of thirty one days per year. The University leave year begins on 1st October. Research staff will normally be expected to take holidays accrued within the leave year. In exceptional circumstances, accrued leave days may be carried forward into the next leave year. Holidays accrued must be taken by arrangement with the Head of Department/line manager within the contract period.

Public holidays to which research staff are also entitled if these days fall within the contract period. Entitlement to public holidays will be as agreed with the institution requirement.

## 7. SICK LEAVE

During any period of absence through illness or injury provided the appropriate medical certificates are received the University will pay a member of staff (having taken account of the aggregate of all periods of absence due to illness during the twelve months immediately preceding the first day of the current absence) as follows:

| **Period of Continuous Employment at commencement of absence from work** | **Full Pay** | **Half Pay** |
|---|---|---|
| Less than 1 year | 1 month | 1 month |
| 1 year but less than 2 years | 2 months | 2 months |
| 2 years but less than 3 years | 4 months | 4 months |
| 3 years but less than 5 years | 5 months | 5 months |
| 5 years or more | 6 months | 6 months |

In order to manage the University's sick pay scheme the University requires to maintain sickness absence records on individual members of staff.

## 8. SALARY

Appointments are made within an appropriate grade of the University's grading structure for Research staff, which is linked to that for academic staff; any nationally awarded enhancements of the grade will be paid. Placing on grade is according to qualifications and experience, and where the post derives from externally provided financial support, to the nature of support. Salaries are payable monthly by means of a credit transfer to a specified bank account.

## 9. PLACE OF RESIDENCE

The University does not normally place specific restrictions upon the place of residence of members of staff. They are, however, expected to reside in a location which is compatible with the satisfactory fulfilment of all the duties associated with their appointment and with membership of the academic community.

## 10. PERIOD OF EMPLOYMENT

Members of staff are employed on the conditions indicated in individual letters of appointment and any accompanying papers. The University is not obliged to give notice of termination or continue any employment beyond the end of that period. Where the period of the contract of employment is for one year or less it may be terminated short of the fixed term period by 1 month's notice on either side. Where the period of the contract of employment is for more than one year, or where there have been a further contract or series of contracts immediately consecutive, the employment may be terminated short of the fixed term period by 3 months' notice on either side.

If the appointment is for a fixed term it will expire at the end of the period without the necessity for notice.

Revised November 2006

**Appendix 3**

University of Strathclyde Glasgow

**Service Commitment to**
**Applicants for Employment**

**Our commitment to you as the applicant is**:

- Your application will be acknowledged *unless stated otherwise in the advertisement* within five working days of receipt. To enable us to meet this, acknowledgement postcards, where enclosed with further particulars, should be completed and returned with your application. Unless otherwise stated in the advertisement, you will also be informed of the outcome of your application as soon as possible.

- If called for interview you will be advised promptly and clearly of the interview arrangements. Your interview will be conducted in a businesslike and friendly manner and will comply with recognised good employment practice. To assist us in meeting our standards we ask that you promptly confirm your attendance (or otherwise) at interview and advise us of any change in your address or Curriculum Vitae.

- You will also be advised of any major delays in the appointment procedure. We will only approach referees nominated by you.

- You will be informed of the outcome of interview as soon as possible. If you are being offered a post you will be written to within 2 working days of the decision being taken. The offer will normally include a duplicate copy which you are required to sign and return to conclude the contract. **Payment of an appropriate salary is dependent on this.**

- We are committed to achieving the standards we have set and to receiving and acting upon constructive feedback from our clients.

- If you are not satisfied with the service you have received, please raise the matter in the first instance with the person with whom you have been dealing. This person will either deal with the complaint to your satisfaction or else advise you how to proceed next. If you feel that dealing with the matter in this way is inappropriate, then write to me at Human Resources, University of Strathclyde, McCance Building, 16 Richmond Street, Glasgow G1 1XQ, and I will respond.

Sandra Heidinger
Acting Head HR

Human Resources
University of Strathclyde
John Anderson Campus
McCance Building
Glasgow G1 1XQ


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**University of Strathclyde**

**Research Fellow**
**Department of Physics**

**(Fixed term to 31 December 2012)**
**Circa 30,000 – 45,000 Euros**

You will participate in a Euratom Framework 7 Support Action on atomic physics for magnetic confinement fusion research in Europe, called ADAS-EU. You will bring to bear special expertise in atomic data, atomic models, spectroscopic diagnostic methods and the plasma environment at Associated Laboratories of the European Fusion Programme and at the up-coming international fusion project ITER.

You will join a team of experts, linked to the ADAS Project, who have for many years engaged in furthering world fusion research and in sustaining forefront atomic physics inputs to it.

This is an exciting and challenging post for an ambitious and dedicated candidate committed to European collaboration and long-term fusion objectives.

You will be based at IPP-Garching, Germany and will also be responsible for travelling to, and supporting, a number of other European labs. The scientific focus will be on beam related issues (emission, attenuation, charge exchange) as well as the atomic physics aspects of the transport and emission characteristics of tungsten.

More information about ADAS-EU and ADAS may be found at http://www.adas-fusion.eu/ and at http://www.adas.ac.uk.

For an application pack visit **http://vacancies.strath.ac.uk** or contact Human Resources, University of Strathclyde, Glasgow G1 1XQ. Tel. 0141 553 4133, quoting ref: JA/R66/2009.

Applications closing date: 6 November 2009.

Some University posts will be subject to a pre-employment Disclosure Scotland Check.

**We value diversity and welcome applications from all sections of the community.**

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# Appendix B

# Travel reports and meetings linked to Dr. Menchero induction and Dr. Guzman annual review

[1] omullane_summary_garching_3-12feb10
[2] planning_meeting_jet_1-12mar10
[3] guzman_talk_jet_3mar10
[4] summary_juelich_7-10Jun10

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# IPP expectations of ADAS-EU post-doc placement

Present : Arne Kallenbach, Thomas Pütterich, Ralph Dux, David Coster
Martin O'Mullane, Luis Menchero
Date : 08 February 2010

Luis Menchero has taken up his position as an ADAS-EU sponsored post-doc at IPP Garching. This meeting was called to discuss areas of interest to IPP which can be addressed in a timely manner as part of this placement. The agenda was open-ended both to give an overview of the breadth of topics to be addressed and to set out the expectations of IPP. It was not intended as a timetable of work but producing a shopping list was difficult to avoid. However such a list is valuable.

Luis is working through the ADAS training course, given at IPP in October 2009, and will undergo further training at JET next month (1-12 March) where the scientific direction for the next 12-18 months will be hardened up. It was felt that it would be useful that the research interests of IPP be discussed as input to this later meeting.

*Items raised at meeting:*

- The ionisation state of the lower stages of tungsten ($W^0$ – $W^{28+}$) is urgently required. Type B, or preferably BBGP, recombination data (with self-consistent prb) will be of immediate benefit to PhD work under way. The possibility of testing against experiment is viable following a similar path as T Pütterich's W cooling factor paper (PPCF, v50, 2008, 085016). The ionisation rates of Stuart Loch are not expected to be exceeded in quality in the near future.
- A set of recommended tungsten data in central ADAS is considered an urgent priority. Comparison with T Pütterich's data before inclusion would be strongly recommended.
- Multiple-step ionisation was mentioned but is not a high priority. D Coster noted that multiple steps fro neutral are simple to implement but multiple steps between more highly ionised ions is a larger programming problem. A 0-D, non-transport, evaluation was considered the best way to proceed if such rates were easily available.
- The ionisation and excitation rates for neutral tungsten are important. Although experimental/empirical S/XB data exists a better theoretical description would be of great interest.
- T Pütterich has extended the Cowan code to deal with very large systems at IPP. He has run the code on the 64Gb TOK cluster. This has recently been upgraded with faster

machines but the modified Cowan code has not been tested. There are trivial differences between T Pütterich's changes and the central ADAS version of the code, principally in labelling choices. Rationalising the IPP and ADAS variants would be helpful. D Coster asked about parallelising the code but its 'old-fashioned' structure may make this task too time consuming. The opinions of an expert in parallel code development would be useful to see if this could be taken further.

- A Kallenbach noted that nitrogen is assuming greater importance in the future fusion programme - in particular JET will probably mandate $N_2$ gas puffing as part of the operating method. The atomic nitrogen data in ADAS is that as assessed by R Dux in 1998. There may not have been much advance in the literature in this period but it should be checked.

- The breakup of molecular $N_2$ is in neutral $N^0$ and $N^+$ is a topical issue in edge modelling. D Coster wished for better cross section data for disassociation and ionisation of $N_2$. D Reiter and F Guzman should be contacted to see whether such data is readily available. R Dux suggested that since the $N^0$ spectrum is easily observed it may be possible to make an AUG experiment to match the atomic, and perhaps molecular band emission, to edge transport simulations thus benchmarking the cross section data.

- There was some concern about the contribution of n=3 (and higher) level of the neutral beam to charge exchange emission. It was suggested that a baseline charge exchange cross section calculation capability would be helpful to answer such questions. Moving a simple CTMC code into ADAS would be helpful.

- The absence of high quality thermal charge exchange data for influencing ionisation balance (adf11/ccd data) for elements other than carbon and hydrogen (and its isotopes) is a limiting constraint on edge transport studies. The 96 data for He is set to zero (L Horton) and the only study to date was carried out for carbon in the mid nineties (C Maggi). Baseline 89 data exists for all elements within ADAS but it is a coarse approximation. Helium is an urgent need with nitrogen and beryllium next. An assessment of the suitability of the 89 data would also be helpful.

- The current minimal maintenance of CXSFIT was not considered to present an immediate problem. However it is a core tool and the lack of upgrading may cause future problems. T Pütterich has commit right to the CVS repository which is hosted on the University of Strathclyde computers. The incorporation of beam modulated signals, for core diagnostics, is the most significant new feature required. A discussion on dealing with modulation in addition to the ELM sequencing, important for edge CX diagnostics, may/will require very machine-programme dependent programming and may not be suitable at this time.

- A new version of CHEAP was discussed briefly. IPP sees the need for a smaller and more flexible code for impurity profile concentration deduction. The consensus was that this is an IPP development without multi-machine capability.

- The simulation of arbitrary spectra, in the context of transport modelling, was raised but no conclusions were drawn. One view, as carried out at IPP, was to generate as

many PECs as required on an as-needed basis. Feature PECs (adf40) were mentioned but the variety of instruments in use, such as spectrometers and diode bolometers, made distributing universal sets difficult. However this is not the way many of the transport code community works. An ADAS spectral prediction code would be desirable but it was not considered to be a high priority task.

- Recommended data, particularly in the ITM context, is a major issue. The clear message is that choice is to be avoided. Having many versions of an atomic database is not a problem but atomic data is seen as just a single input. From an ADAS perspective the number of data types required is modest. Selecting one adf11 set for each element and an ITM set of photon emissivities, modelled on the adf15/transport set, would satisfy the current need. In particular the splitting of useful carbon PECs over 'pju' and 'vsu' files has resulted in the 93 data remaining in use. It was noted that transition selection is performed on wavelength. A document listing the recommended adf11 and adf15 data is urgently required. The ITM data extraction and generation should be automated and updated at each ADAS release.

- Error estimation was another topic of interest and the atomic coefficients are seen as an entry to propagating error through the transport codes. It was agreed that ADAS could supply coefficients with error surfaces and a pilot programme to explore errors be started.

*Other issues raised outside the meeting:*

- Prof. Behringer met with Luis and offered to mentor him with particular emphasis on the requirements of interpreting measurement from tokamak plasmas.

- The incorporation of ADAS neutral beam data into FAFFNER and TRANSP is proceeding well. However Michael Kraus has finished his diploma thesis and is moving on to other fields, although he will be available for consultation. Two outstanding issues need to be addressed. Firstly helium, as a stopping rather than diagnostic species, is required. A similar approach to generating a large dataset via *run_adas310.pro* will be performed with *run_adas311.pro*. The metastables will be considered to be in equilibrium. Secondly the assumption that ion and electron temperature are the same introduces unnecessary discrepancies for highly unequal temperatures. A correction for ratios varying from 0.1 to 10 of Te/Ti will be added.

- The production of coefficients which separation the charge exchange and ionisation processes follows the CHEAP approach whereby the an effective stopping coefficient calculated with ion impact processes switched off is subtracted from the full coefficient, thus preserving the multi-step physics. The capability to control this via options to *run_adas310.pro* (with interactive ADAS following later) rather than recompilation should be advanced. Negative values were found at the extremes of the plasma parameter range considered. M Kraus will report on these parameters when he returns from his holiday.

- Missing physics when calculating radiated power, particularly for filtered or restricted energy ranges, as found in bolometers/soft x-ray diodes. is an outstanding issue. For those ionisation stages which are limited in the number of configurations that can be included in an adas801 calculation the configuration-average top-up may still be insufficient. A further, bundle-n top-up was discussed and should be explored.

- adf11 data for the ecd, ycd and zcd classes for 89 and 96 data has been added to central ADAS at IPP and JET to allow various bundling schemes to be explored.

ADAS-EU planning meeting
JET Facility/Culham Laboratory
1-12 March 2010

*Participants:* Alessandra Giunta, Francisco Guzman, Stuart Henderson, Luis Menchero, Christopher Nicholas, Martin O'Mullane, Hugh Summers.

*Agenda:*

| | | |
|---|---|---|
| *Mon 1 Mar:* | 09.30-10.30 | Personal – email etc |
| | 10.30-12.00 | Admin. Matters – computer accounts |
| | | Lunch |
| | 13.00-14.00 | JET/MAST walk round |
| | 14.00-16.30 | ADAS-EU workplan review |
| *Tue 2 Mar:* | 08.30-9.30 | Personal time – email etc |
| | 09.30-12.00 | Topic based joint scientific discussion – GCR/Special features |
| | | Associated development/work identification |
| | | Lunch |
| | 13.00-14.00 | Personal time – email etc |
| | 14.00-16.00 | Topic thinking through/getting up to speed |
| | | Binary discussions with HPS and MOM |
| | 16.00-16.30 | Topic summary discussion |

*Wed 3 Mar:* as for Tue 2 Mar – topic Molecules. Francisco Guzman talk 14.00-14.30

*Thu 4 Mar:* as for Tue 2 Mar – topic Beam stopping and Emission.

*Fri 5 Mar:* as for Tue 2 Mar – topic Charge exchange spectroscopy.

| | | |
|---|---|---|
| *Mon 8 Mar:* | 08.30-9.30 | Personal time – email etc |
| | 09.30-12.00 | Topic revisit – GCR/Special features |
| | | Focusing on tasks/workpackages, scheduling, assignment of tasks, assignment of report responsibility |
| | | Lunch |
| | 13.00-14.00 | Personal time – email etc |
| | 14.00-14.30 | Luis Menchero – overview talk of research activities |
| | 14.30-16.00 | Topic thinking through/getting up to speed |
| | | Binary discussions with HPS and MOM |
| | 16.00-16.30 | Topic finalizing discussion |

*Tue 9 Mar:* as for Mon 8 Mar – topic Molecules.

*Wed 10 Mar:* as for Mon 8 Mar – topic Beam stopping and Emission.

*Thu 11 Mar:* as for Mon 8 Mar – topic Charge exchange spectroscopy.

| | | |
|---|---|---|
| *Fri 12 Mar:* | 08.30-9.30 | Personal time – email etc |
| | 09.30-12.00 | Visits, next meeting, ADAS-EU Course, ADAS Workshop, Conferences. |

HPS
1 Mar 2010

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# Molecular ADAS: Status Report.

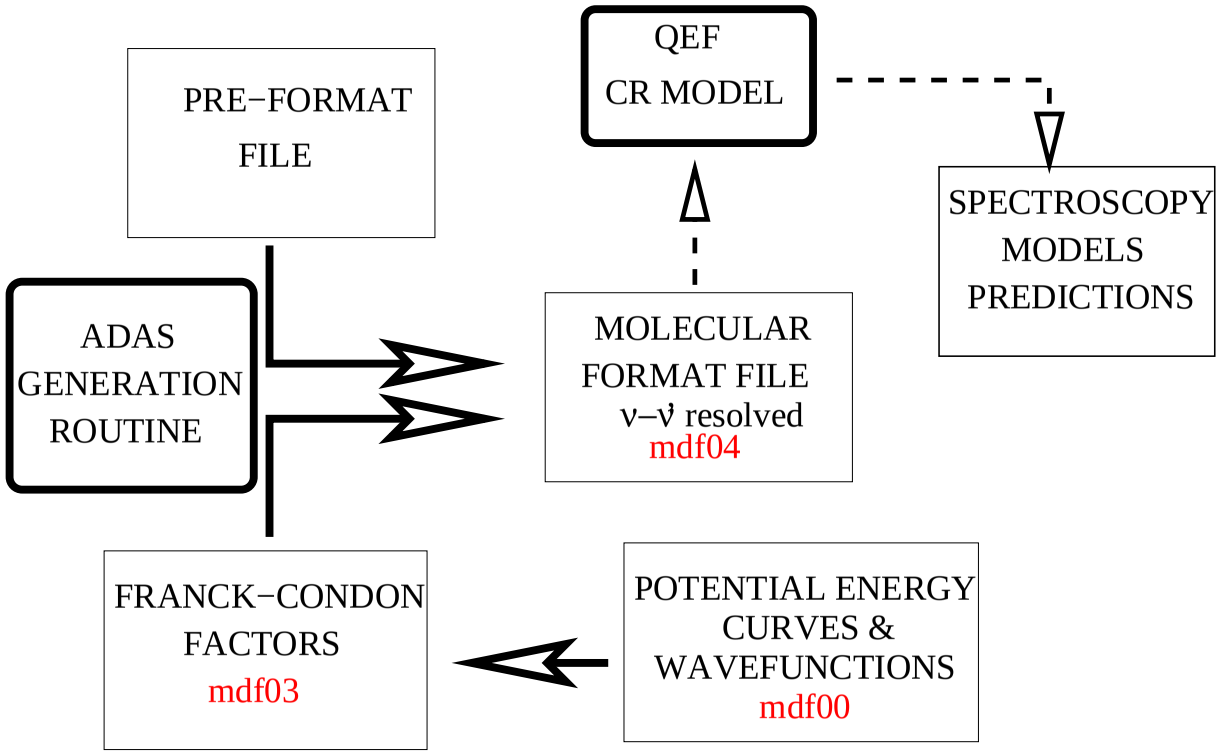
Francisco Guzmán

ADAS-EU
University of Strathclyde

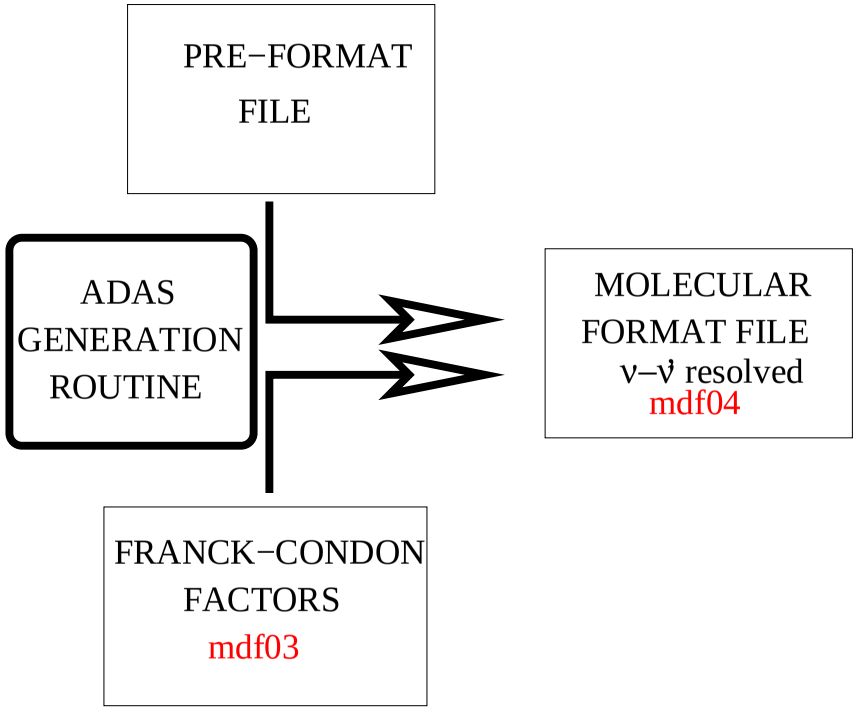
March 3, 2010

# Outline

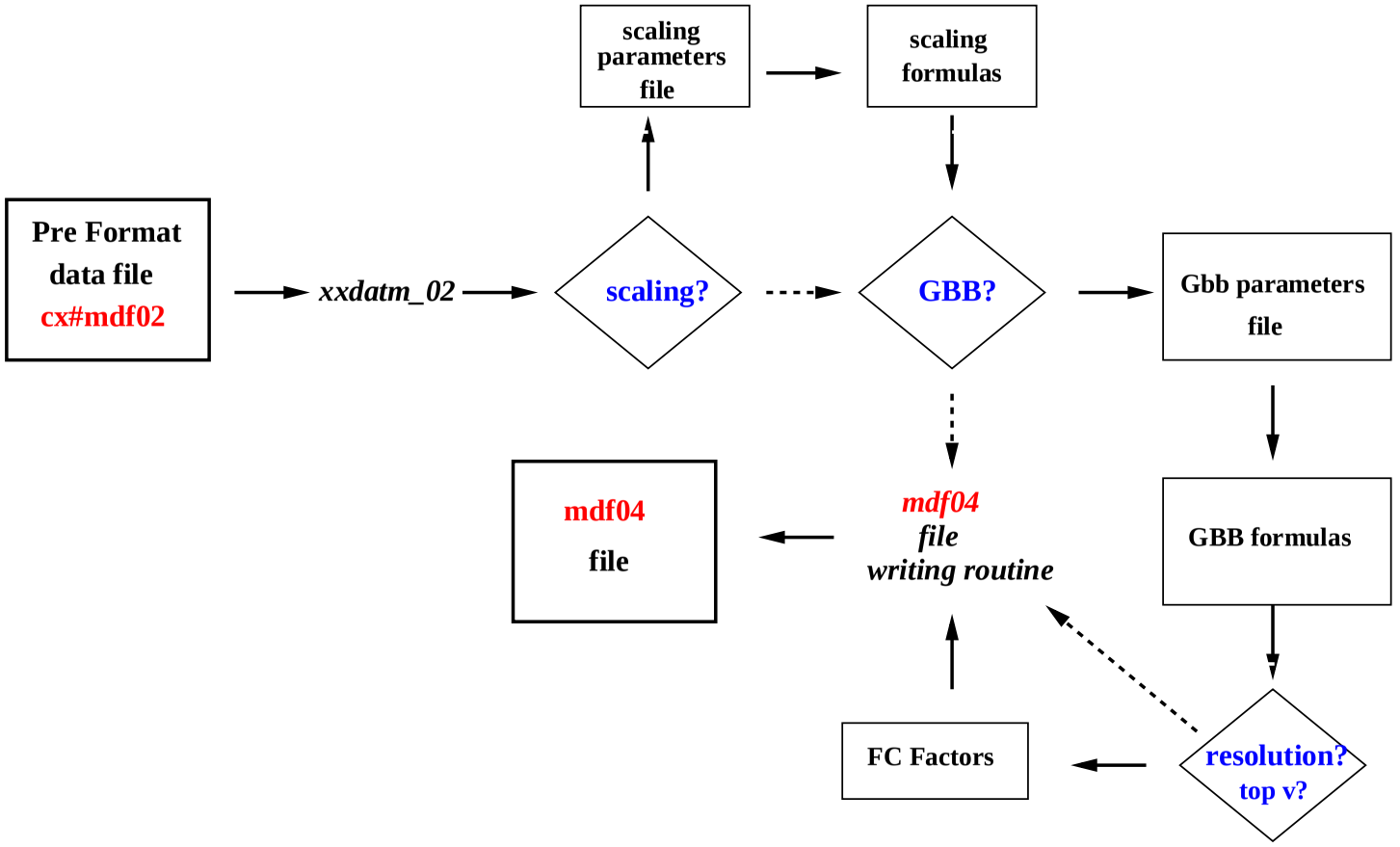
# *mdf* Series


QEF
CR MODEL
PRE−FORMAT
FILE
SPECTROSCOPY
MODELS
PREDICTIONS
ADAS
GENERATION
ROUTINE
MOLECULAR
FORMAT FILE
v–v' resolved
mdf04
FRANCK−CONDON
FACTORS
mdf03
POTENTIAL ENERGY
CURVES &
WAVEFUNCTIONS
mdf00

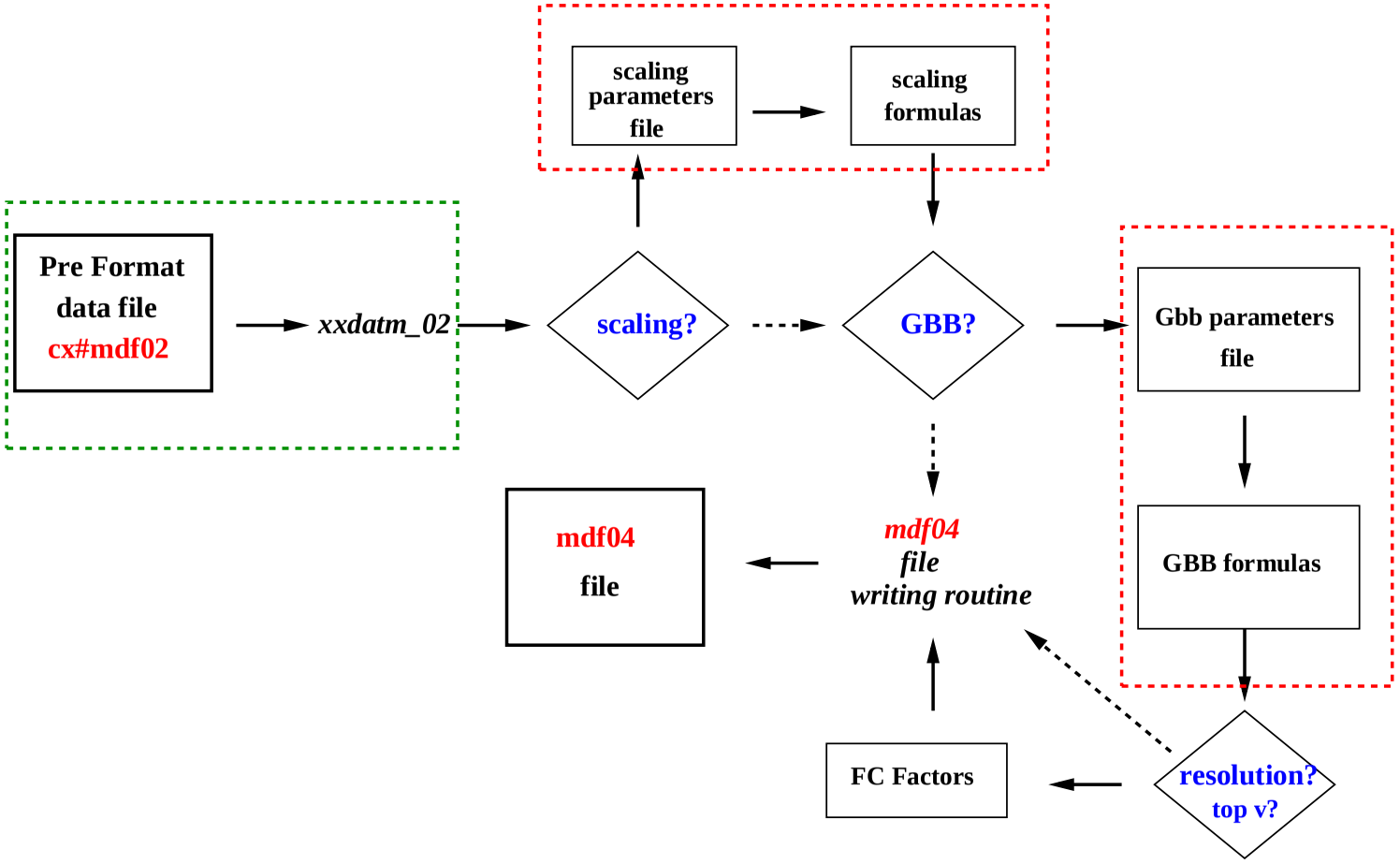
# *mdf* Series


PRE−FORMAT
FILE
ADAS
GENERATION
ROUTINE
MOLECULAR
FORMAT FILE
ν–ν′ resolved
mdf04
FRANCK−CONDON
FACTORS
mdf03

# Generation of mdf04



# Generation of mdf04



# Pre Format File: *cx#mdf02*

- Pre Format file (*mdf*02) is a compilation (from Janev) of available **cross sections** data already present in the literature.
- Only data with calculations or experimental background is included in *mdf*02. Scaled data could be generated after depending of the choice of the user.
- Due to the big size of the files each specie processes will have its own pre-format file:
  cx#mdf02_h2.dat for $H_2$
  cx#mdf02_h2p.dat for $H_2^+$
  cx#mdf02_h2m.dat for $H_2^-$ (if needed)
  cx#mdf02_h3m.dat for $H_3^+$ (if needed)

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# Format: Molecular Indexes

indx_s Different molecular and atomic species.

indx_p Different process departing from a specie.

indx_e Different electronic states of each specie.

indx_v Vibrational index for each electronic state.

indx_r (internal) Reactions from one electronic state of one specie to another different specie or/and electronic state.

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# Pre format file:*cx#mdf02_h2*

```
H_2        / electron impact                                                mdf
/
species
/-------
/ ind_s   identity   e-config    e-coupling   ch_ion   bwno_i       ch_dis      bwno_d
/ -----   --------   --------    ----------   ------   ------       ------      ------
   1       H_2        dia-ua      dia-term     1->2    124418.       1->4+4    36117.00
   1       H_2        dia-ua      dia-term     1->2    124418.       1->5+6    36117.00
   2       H_2^+      dia-ua      dia-term     2->5+5    5386.       2->4+5    21380.21
   3       H_2^-      dia-ua      dia-term     3->1         0.       N         00000.00
   4       H          atm         atm-term     4->5    109691.       N         00000.00
   5       H^+        atm         atm-term     N            0.       N         00000.00
   6       H^-        atm         atm-term     6->4       427.       N         00000.00
/
process
/-------
/
/ind_p                          path                                  description
/----- ------------------------------------------------------   --------------------
   1   e+H_2(v=0) -> H_2^-(X(2)S(+)(u),B(2)S(+)(u)) -> e + H_2(v') vib exc via e attach
   2   e+H_2(v=0) -> e + H_2*(1)N                                 vib unr. exc.-> singlet
   3   e+H_2(v=0) -> e + H_2*(3)N                                 vib unr. exc.-> triplet
   4   e+H_2(v) -> e + H_2*(1)N                                   vib unr. exc.-> singlet
   5   e+H_2(v) -> e + H_2*(3)N                                   vib unr. exc.-> triplet
   7   e+H_2(v) -> e + H_2*(1)N -> e + H(1s) + H(nl)              vib unr. diss. exc.-> singlet
   8   e+H_2(v) -> e + H_2*(3)N -> e + H(1s) + H(nl)              vib unr. diss. exc.-> triplet
   9   e+H_2(v) -> e + H_2*(1)N(v')                               vib res. exc. -> singlet
  10   e+H_2(v) -> e + H_2*(3)N(v')                               vib res. exc. -> triplet
  11   e+H_2*(N(v)) -> e + H_2*(1)N'(v')                          vib res. exc. -> singlet
  12   e+H_2*(N(v)) -> e + H_2*(3)N'(v')                          vib res. exc. -> triplet
  13   e+H_2(N(v)) -> e + e + H_2+(2)                             vib unr. ion. to ground state
 ...
```

# Pre format file:*cx#mdf02_h2*

```
states
/------
/ ind_s  ind_e   e-con-ua  e-con-sa   coupled state   (wt.-1)/2
/ -----  ------  --------  --------    -----------    ---------
   1       1     1ssg1ssg    1s1s       (1)S(+)(g)        0.0
   1       2     1ssg2ssg    1s2s       (1)S(+)(g)        0.0
   1       3     1ssg2psu    1s2p       (1)S(+)(u)        0.0
   1       4     1ssg2ppu    1s2p       (1)P( )(u)        1.0
   1       5     1ssg3ssg    1s3d       (1)S(+)(g)        0.0
   1       6     1ssg3psu    1s2s       (1)S(+)(u)        0.0
   1       7     1ssg3ppu    1s3d       (1)P( )(u)        1.0
   1       8     1ssg3dsg    1s2p       (1)S(+)(g)        0.0
   1       9     1ssg3dpg    1s3d       (1)P( )(g)        1.0
   1      10     1ssg3ddg    1s3d       (1)D( )(g)        2.0
   1      11     1ssg4ssg    1s3p       (1)S(+)(g)        0.0
   1      12     1ssg4psu    1s3s       (1)S(+)(u)        0.0
   1      13     1ssg4ppu    1s4p       (1)P( )(u)        1.0
   1      14     1ssg4dsg    1s3d       (1)S(+)(g)        0.0
   ...
```

# Pre format file:*cx#mdf02_h2*

- The variable *numer* indicates if numerical data are available (n. of entries) or not (0).
- Numerical values will be filled while the formula index *form* (form=0 -> no formula provided) will give the fitting formula in which the parameters *par_val* are used.

```
/ch_in           ind_p        ch_out      ch_dis
/-----          ------        ------      ------
s   e   v                    s   e   v
1   1   0        1           1   1   1
                      parameters & values
                      -------------------
categ=1  tcode=3  a_val=0.00e+00  a_dis=0.00e+00  form=1   par=1  numer=27  DE=0.516e+00
     te=  0.5160       0.7000       0.9000       1.000       1.200       1.400       1.600
           1.800       2.000        2.200        2.400       2.600       2.800       3.000
           3.250       3.500        3.750        4.000       4.500       5.000       5.500
           6.000       6.500        7.000        8.000       9.000       10.00
    omg=   0.000       0.9443E-04   0.4522E-02   0.1189E-01  0.3984E-01  0.8156E-01  0.1299
          0.1790       0.2252       0.2668       0.3031      0.3340      0.3601      0.3816
          0.4031       0.4195       0.4316       0.4403      0.4496      0.4515      0.4484
          0.4422       0.4340       0.4246       0.4042      0.3834      0.3633
par_val=   1.0000e+00
```

# Pre Format File: *cx#mdf02_h2*

- **Excitation data** The avalaible data have been checked to be in good agreement with the fitting formulas.
- **Ionization data** Checked as well. Only ionization from ground state. Ionization from excited states can be achieved using Grycinski model.
- **Attachment** Formulas from Celiberto for DA fitting calculations. Vibrational excitation through resonant attachment.

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- **Dissociation + Ionization** No fitting formulas (for cross sections). Available calculations from Atems and Wadehra and Celiberto (Celiberto contacted by email).
- **Double excited** There are not cross sections calculation. Contribution small to photoionization ($\sim$5%). No information in cross sections for autoionization.
- **Predissociation** Only rates available. Can be a significant branching ratio. CR model??
- **Metastable** Only excitation and attachment data (no ionization) available.

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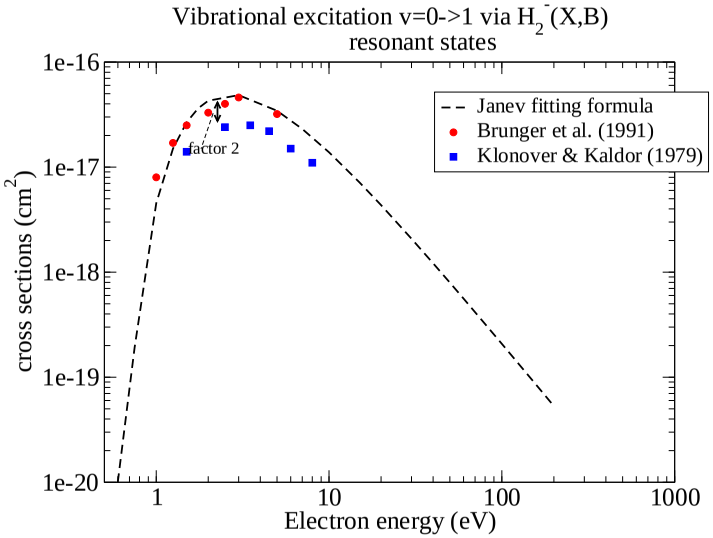
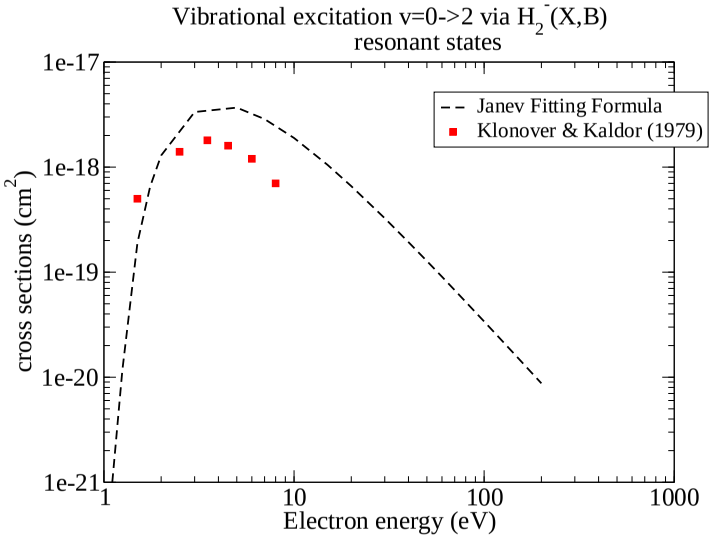
# Fitting vs. numerical data

## Excitation data

The fitting formula try to get a continous asymptotic behauviour from the numerical data choosing the most reliable sets of data in each energy range and each process.

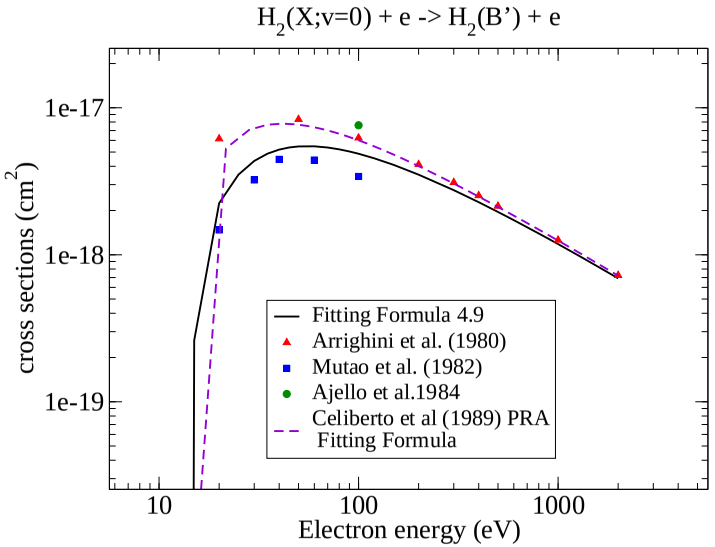


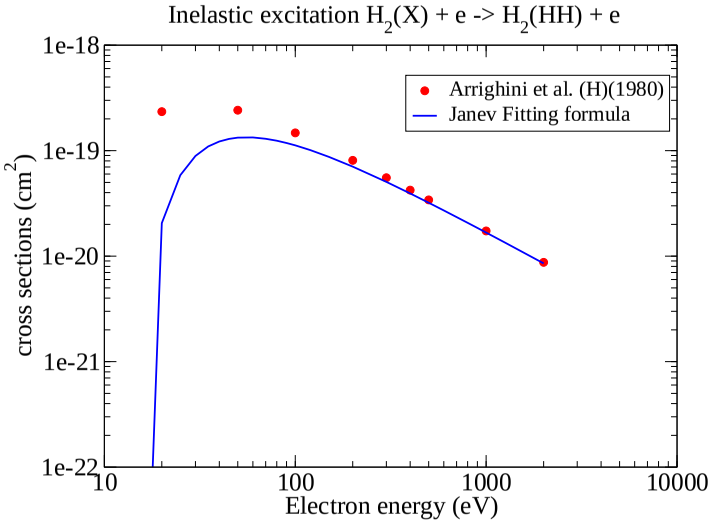



# Fitting vs. numerical data

## Excitation data

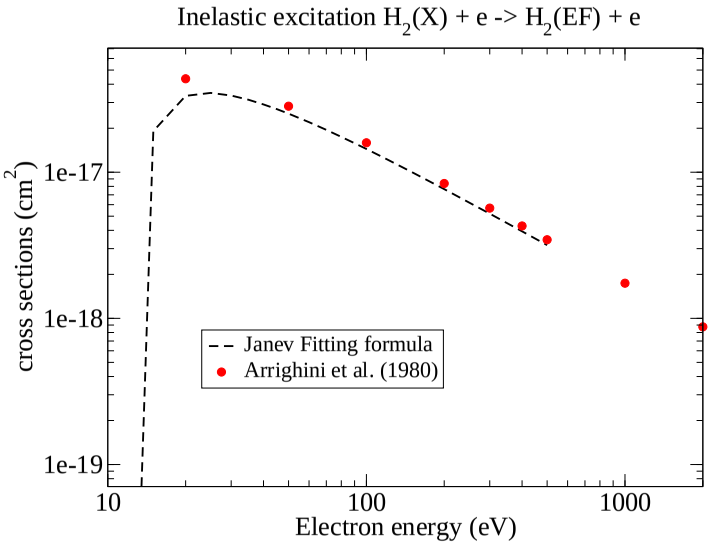
Sometimes a compromise between the different data and the correct beahauviour is adquired.

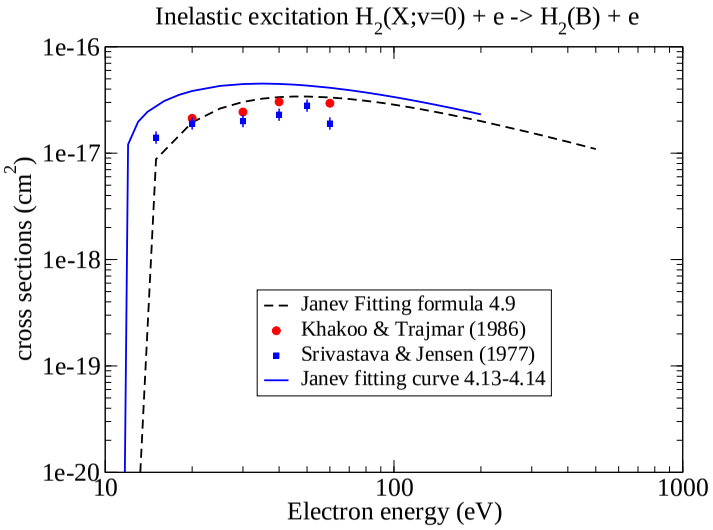


# Fitting vs. numerical data

## Excitation data

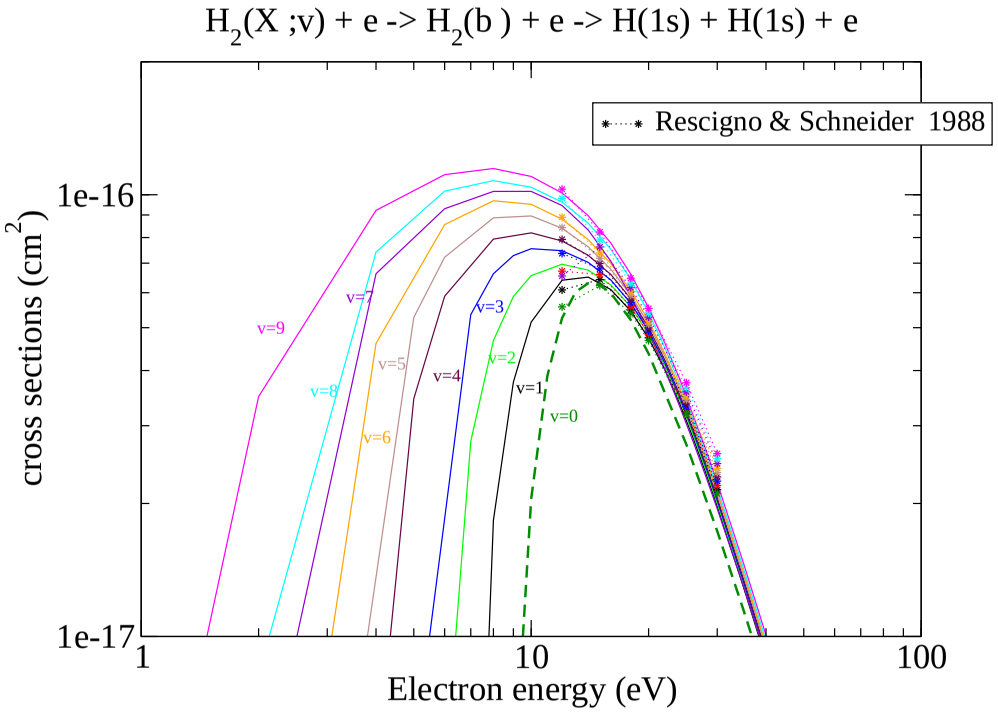


# Fitting vs. numerical data: dissociation through $b^3\Sigma_u^+$

## Excitation data

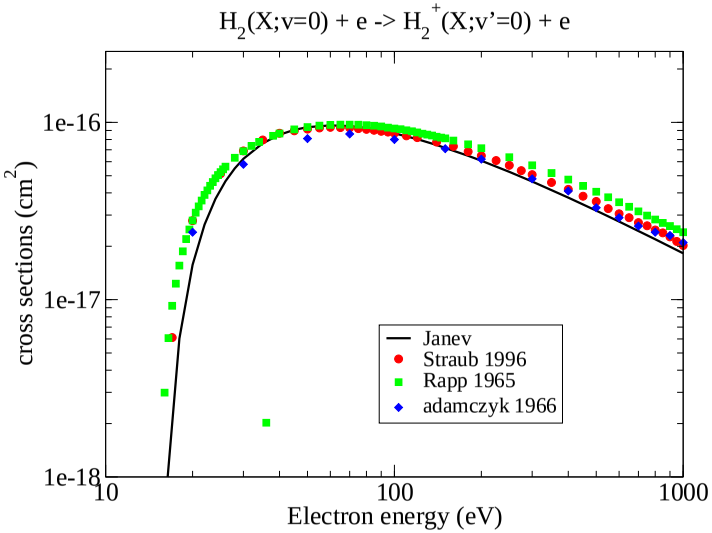
All the population that goes to $b^3\Sigma_u^+$ dissiociative channel contributed to dissiociation.

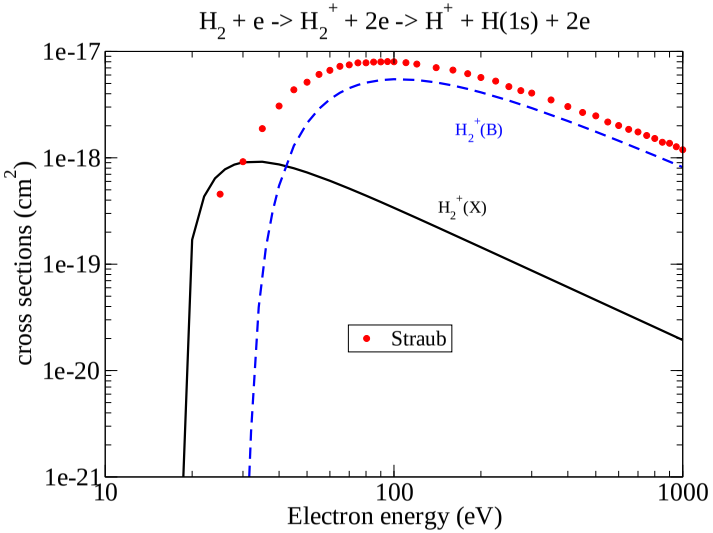


# Fitting vs. numerical data

## Ionization data

- Non dissiociative ionization cross sections only avalaible from ground state of ion.
- Vibrational resoved cross section trough FC scaling and from excited states GBB modelling.

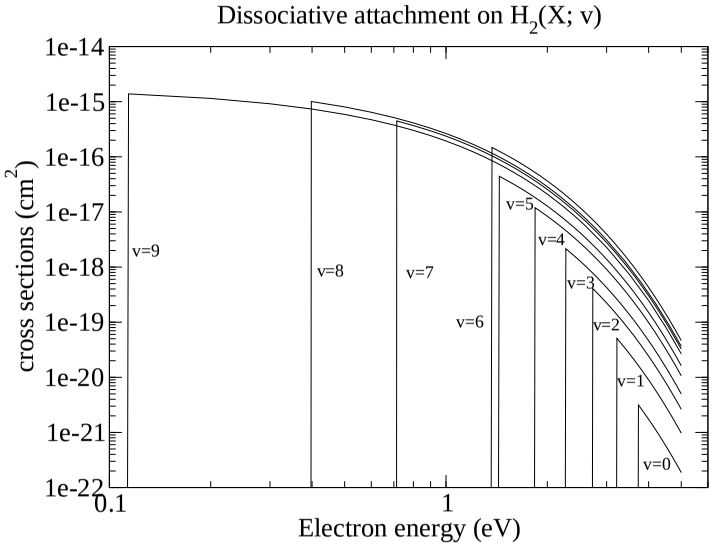


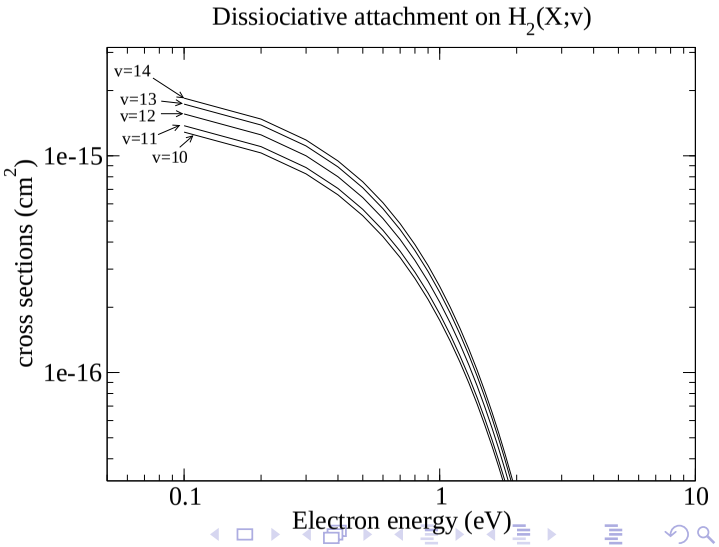



# Fitting vs. numerical data

## Dissociative Attachment data

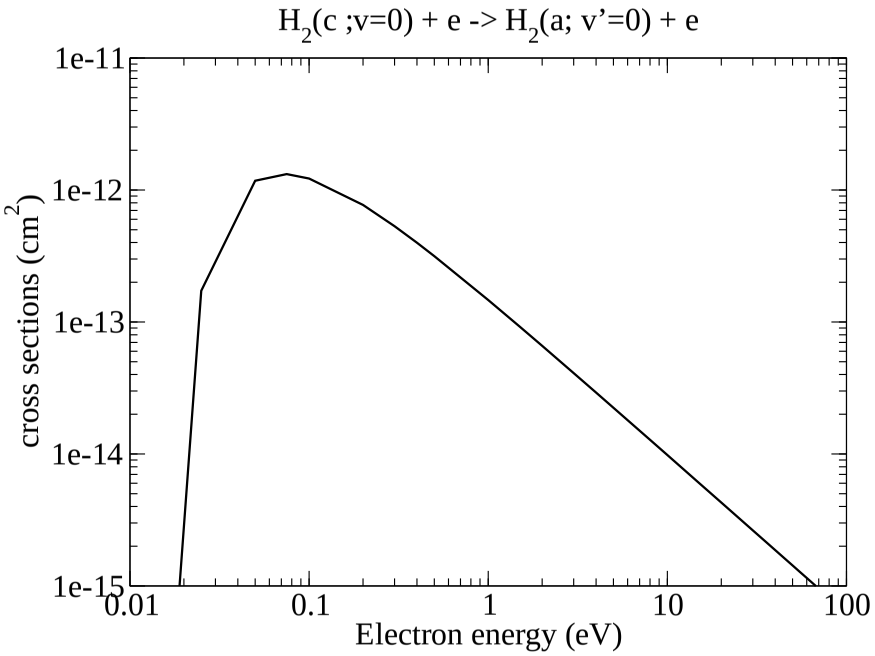
- DA has relative high cross sections and exhibits a pronounced isotope effect. Could it be scaled??
- However, this ocurrs in a small range of energies and can be neglected beyond 5eV.
- Big values could take place for DA from excited states, only estimations available from simple modelling.



# Metastable ($c^3\Pi_u; \nu = 0$); $\tau \sim$ 1ms

- The metastable has a big coupling with $a^3\Sigma_g^+$ state with a high excitation cross section.



# Metastable ($c^3\Pi_u; \nu = 0$); $\tau \sim 1$ms

- Cross sections to ($a^3\Sigma_g^+; \nu$) can be scaled with FC factors.
- Other excitations from metastable are 3 or 4 orders of magnitude smaller. Janev conclusion is that process of excitation to $a^3\Sigma_g^+$ is the only important process. Nevertheless, there are other excitation published data in the literature.
- Ionization not avalaible (can be (over)estimated by GBB). DA can be modelled in a quasi-classical aproximation.

# Collisional Radiative tasks to do

1. Ion impact cross sections and FC factors will be compiled (around 1-2 months). Needed bound-unbound transition FC factors (Schneider?). Not consider $H_3^+$ and molecule collisions (important for linear machines)?? Neutral-molecules??
2. Radiative data must be compiled or calculated by means of Janev work. Assuming plasma is optically thin only radiative coefficients needed.
3. Maxwellian rates should be calculated. ADAS routines???
4. Coupled equations will be solved like in atomic case.
5. Various levels of resolution could be achieved.
6. Rates can be tested in spectroscopy experiments. (desirable)

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# Conclusions

- Excitation data seem complet save for the collisional transition between electronic states.
- Ionization calculations from excited state would be desirable. Autoionization data can be important as well. Ionization from metastable required.
- DA could not be important at intermediate-low plasma energies but dependence with density and process time has to be checked.
- Predissociation mechanism can be important. Need to account for it in CR models.

# Conclusions II

- Ion impact data in progress. Should be incorpored in CR together with electron impact.
- Isotopes as $D_2$, HD, $T_2$, DT and HT could be treated separately. Scaling the fitting formulas??
- A revision of data will be done in parallel with the developping of CR model and new data could be added.

-

# ADAS-EU Travel Report

*Location:* Institute for Plasma Physics, Forschungzentrum Jeulich, Germany.
*Date:* 8-9 Jun 2010.
*ADAS-EU staff:* Hugh Summers.
*Persons visited:* Francisco Guzman, Ratko Janev

*Items:*

(1) Dr. Guzman, the ADAS-EU PDRA placement at Fz-Juelich, has now been in post for eleven months. It was appropriate to have the 'home base annual review', scheduled in the ADAS-EU proposal, in advance to coincide with the induction/training of Dr. Menchero. The third strand of the ADAS-EU external staffing arrangements is the employment of Professor Ratko Janev at 10% FTE for two years. It was agreed that for the first year of Prof. Janev's appointment, that it should be implemented as one month, full time, at FZ Juelich to allow effective overlap and engagement with Dr. Guzman. The delayed start date of Dr. Guzman's appointment (1 Jul 2009) made this impossible in 2009, so Prof. Janev's engagement was pushed back one year. Prof. Janev's appointment was successfully implemented by Human Resources, Strathclyde University on 1 Jun. 2010 as one month full-time for 2010. The present visit by Prof. Summers serves a dual purpose of discussing and initiating the ADAS-EU work of Prof. Janev and assessing the effectiveness of the engagement of Dr. Guzman with FZ Juelich after one year.

(2) First discussions centred on the molecular hydrogen database and progress towards its inclusion in ADAS. Francisco explained his approach with precursor datasets (*mdf02*) which are composed of reaction cross-sections between electronic states and the resolved data sets which are vibrationally resolved. The mapping from the first to the second uses a combination of tabulated and internally calculated Frank-Condon factors. It has already been agreed that new ADAS data formats are required for the molecular case and that these should be called 'molecular data formats', such as *mdfnn* similar to the older data formats for atoms and ions of the form *adfnn*. These will parallel as far as possible the catagories of application, so that *mdf04* is formally equivalent to *adf04* allowing a population structure calculation for molecular states in the former case.

(3) At issue is the completion of the transfer of all relevant data into the mdf04 files ensuring that they are as complete and well validated as possible. The assembled background source is the compilations of Ratko, the most complete and up-to-date of which is nearing completion as a book (authors, Reiter, Janev and Samm). ADAS requirements for *mdf* includes both numerical and fitting formula representations. In some cases, the existence of a single preferred numerical curve (Janev imprimateur) is not available, so the task has expanded with some re-verification of sources and preferred curves. This is a shared task at FZ Juelich involving Francisco, Ratko and Detlev. Some ion impact processes are missing, but are needed for the molecular collisional-radiative models. Simple approximations for these, such as Grysinski's formulae and results derived via Summers' IPPROG are not sufficiently secure. Ratko will reassess these as part of his efforts.

(4) It is noted that Francisco has transfered first stage *mdf02* and the associated *xxdatm_02.for* reading routine to Martin for inclusion in central ADAS at the next release. Under consideration is a new ADAS series for the molecular work, *adas9xx*, and when this should scheduled for first release and what its first content should be. Hugh pointed out that the cross-section to rate coefficient conversion (*mdf02* to *mdf04*) with asymmetric distribution functions should be considered again with fresh eyes, with the hindsight of EIRENE and ADAS experience.

(5) The objective of an ADAS basic molecular collisional-radiative code, as a pedagogical tool and as a route to data checking and completeness examination, met with approval. Hugh is keen that first steps on setting up the collisional-radiative model should be done soon. Even if just vibronic $H_2$ at this stage, it would reveal modelling issues which might impact data archiving early. Ratko pressed the need to handle $H_3^+$ . This is in the context of the discharges which are the sources for neutral beams primarily and is an area which we wish to be within ADAS capabilities. The non-linearity introduced by $H^+$ and H in collisions for the collisional-radiative models is an issue. Again Hugh felt that early pilot studies were important there too.

(6) There was discussion on other CXS issues, although the existing ADAS-EU activities span the most direct problems. It was felt that Ratko's insight on scaling laws for collisions

would be advantageous for refinement of the baseline efforts in ADAS for arbirarily heavy and highly charged ions.

(7) In separate discussions, Francisco and Hugh considered the generality of questions generated within FZ Juelich with which ADAS could connect. The modelling of transient radiated power in disruption mitigation has been posed . This would involve gases such as nitrogen. Francisco proposed initial modelling using the basic transient code *ADAS406* as a start. As the key personnl at FZ Juelich were absent, it was not possible to for Hugh to participate in immediate follow-up. The derived data in ADAS, especially *adf11* is satisfactory for these purposes, but the *ADAS406* model may be too limited. Further detail on the evolution of electron temperature and density and the spatial movement and spreading of the gas plume emission was required to make progress. Francisco will pursue this.

(8) Neutral and singly ionised tungsten remains a main focus at FZ Juelich. ADAS-EU has taken steps to speed up assembly of its efforts on this question. It is expected that our University of Mons-Hainaut collaborators will have the optimised Cowan intermediate (rcn) files for running through Martin's post-processing by Aug. 2010. At that point re-engagement with the experiments and REO modelling will be possible. Francisco will act as the link and monitor the developments.

(9) Hugh and Ratko discussed the location and timing of Ratko's ADAS-EU engagement in 2011. Hugh felt, that with the molecular collisional-radiative models expected to be on stream in 2011, that the month would profitably be spent at Culham Laboratory/JET. Ratko concurred if arrangements can be made. Tentatively, April or May 2011 will be aimed for.

(10) Francisco is working assiduously at FZ Juelich and the predefined tasks are progressing, albeit more slowly than originally planned. The embedding of molecular data in ADAS., preserving ADAS-type pedagogical and modelling links is more time consuming than expected. The conversion of reaction tabulations from book form to ADAS computer system form requires substantial effort. Nonetheless there is no doubt the work package will be achieved in due course.

(11) Intercommunication between the Francisco and staff at FZ Juelich is not developing as quickly as hoped for. It is difficult to predict a pace for this, but the rather independent working of sub-groups at FZ Juelich, seems to be a factor. Also a loss of some strong spectroscopic leadership from FZ Juelich has had an effect. By and large progress is acceptable and certainly the pre-defined tasks, because of the presence of Prof. Reiter and Prof. Janev at FZ Juelich are themselves an adequate justification for the FZ Juelich placement.

HPS
28 Jun 10

# Appendix C

# Sub-contracting set-up visit reports and sub-contracts

[1.1] summary_vienna_24feb10
[1.2] contract_vienna_8jun10
[2.1] summary_vilnius_31mar-1apr10
[2.2] contract_vilnius_5jul10
[3.1] summary_belfast_25mar10

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ADAS-EU Travel Report

*Location:* Institute fuer Allgemeine Physik, Technical University, Vienna.
*Date:* 24 Feb 2010.
*ADAS-EU staff:* Hugh Summers.
*Persons visited:* Professor Friedrich Aumayr, Ms Katherina Igenbergs.

*Items:*

(1) Discussion centred on establishing an ADAS-EU subcontract with the Technical University, Vienna. This would be to place relevant atomic data for neutral lithium and neutral sodium beam diagnostic models of magnetic fusion plasma into ADAS and possibly also pedagogical versions of the diagnostic modelling codes.

(2) It was noted that TUW had a long history of effort on the neutral lithium beam diagnostic and more recently with efforts on a matching capability for neutral sodium beams. These activities are conducted in close collaboration with IPP Garching and Dr Josef Schweinzer. In particular, Katerina is located in Munich and spends substantial periods of time connected with the lithium beam diagnostic at IPP Garching.

(3) Professor Aumayr now heads the Atomic and Plasma Physics Research Group at TUW following the untimely death of Professor Winter. The Group continues its momentum in the beam area of magnetic confinement fusion and in the generation of relevant ion impact, especially charge exchange data.

(4) Professor Summers reiterated the intention and wish, proposed and endorsed by IPP Garching and TUW when the ADAS-EU plan was in development, that the lithium and possible sodium beam data base should be incorporated and maintained in ADAS. He pointed out that, at that time, the diagnostic methodology was in an established state and long term maintenance in ADAS seemed desirable by all parties. However development has resumed, especially by Dr Schweinzer in new Bayesian methods and codes for the lithium beam analysis, and so the merit and value of an ADAS role needed to be re-evaluated.

(5) Professor Aumayr drew attention to the group's published work in the atomic database area, including At. Data and Nucl. Data Tables (1999), 72, 239 for the lithium beam and At. Data and Nucl. Data Tables (2008), 94, 981 for the sodium beam.

(6) The widespread use of the lithium beam diagnostic at fusion laboratories was noted. Professor Summers enquired about the expected role for the sodium beam. Professor Aumyr explained that the hoped for expansion of the parameter range (electron temperature and density) through altered penetration and excitation of the sodium beam compared with the lithium beam had not been realized. The effects countered each other and so the sodium beam essentially duplicated the scope of the lithium beam. Thus, in the medium future, further development of the sodium beam diagnostic is not planned.

(7) Professor Aumayr explained that the database and the diagnostic analysis codes for both the lithium and sodium beams had been developed at TUW. These codes were now in a frozen state with new code development at IPP as mentioned in (4) above. On the other hand, theoretical fundamental cross-section calculation at TUW had increased with the studies of Katherina and so in some ways TUW activities had moved closer to ADAS.

(8) Professor Summers pointed out that Professor Ratko Janev would be employed part time by ADAS-EU for two years. Prof. Janev, while at IAEA, worked closely with Prof. Winter on the ion impact data for the lithium beam. This opens the possibility of his participation in assessment and update of the lithium and sodium databases if they are incorporated in ADAS.

(9) Katherina, in her PhD activities, has been working with Dr. Schweinzer on state-selective charge exchange cross-sections for hydrogen collision with impurity nuclei in the CCAO approximation. Recent work includes $Be^{+4}$ + H(n=1,2) ( J.Phys. (2009, 42, 235206) and $O^{+8}$ + H(n=1,2). She has been extending the number of states addressable by the CCAO codes (originated by the Oslo group with the participation of Dr Schweinzer) and moving the codes onto multi-processor supercomputers with the visible transitions of $Ar^{+18}$ as the target. Codes are being modified and tested for this extension but the $Ar^{+18}$ study has not yet been completed.

(10) Professor Summers pointed out the relevance of Katherina's work and its strong complementarity to the CCMO and Monte Carlo capabilities of the ADAS-EU staff (and their links to the UAM Madrid activities in support of ADAS and ADAS-EU). Professor Summers also emphasized the importance of the ion impact excitation cross-section data

for the hydrogen atom projectile for consistency and completeness of the beam stopping/beam emission and charge exchange spectroscopy.

(11) It was noted that Katherina would complete her PhD activities at TUW in around one year. She would be the most suitable person at TUW to implement any ADAS-EU sub-contract with TUW, so sub-contract timing should recognize this.

(12) It was generally agreed that it would be straightforward to convert the lithium and sodium databases to suitable ADAS formats (or re-defined formats) and to create the necessary access subroutines/procedures. Also that Katherina's data could be easily completed (as in (10) above and routed into ADAS formats.

(13) Professor Summers pointed out that ADAS is not simply a database but rather a modelling and analysis infrastructure. Also, interactive ADAS has many codes which allow pedagogical exploration of collisional-radiative models and their diagnostic potential. Thus, although the actual lithium beam diagnostic implementation (and codes) at IPP Garching and elsewhere would be outside the scope of ADAS, the TUW frozen lithium/sodium code might easily adapt for ADAS in a pedagogical role as above.

(14) In summary, Professor Summers and TUW felt there was valuable material, appropriate scope and enthusiasm at TUW to work-up a sub-contract on the basis of the above notes and discussions. Professor Summers will engage to prepare a draft scientific annex for an ADAS-EU sub-contract as soon as possible for further discussion - recognizing the above staff/time constraints.

HPS
6 April 2010

# ADAS-EU CONTRACT

ATOMIC DATA AND MODELS FOR NEUTRAL BEAM DIAGNOSTICS.

(1) LITHIUM AND SODIUM BEAM MODELS AND DATA.
(2) CCAO CALCULATIONS FOR H (N=1,2) TARGETS.

H. P. Summers

8 June 2010

## 1. Summary

It is proposed to contract with Prof. Friedrich Aumayr, Institute of Applied Physics, Technische Universität Wien, Vienna, Austria to make available in ADAS a comprehensive set of atomic rate coefficient data for the use of neutral lithium and sodium for beam diagnostics. These relate to processes determining the state of excitation of the beam species and to its action as a donor to plasma impurity ions. The TU Wien group will assist ADAS-EU staff in installing a pedagogical tool within the interactive IDL-ADAS system as a guide to the diagnostic method and to assist in data verification and maintenance. Additional theoretical state selective charge exchange data in the CCAO approximation for neutral hydrogen as a donor to selected full stripped impurities in the nuclear charge range 4-18 will be added to the ADAS database. In association with ADAS-EU staff, these latter data will be merged with other data in the ADAS database to provide new preferred data collections for application.

The work will make extensive use of the methods and codes developed by Prof. Winter, Prof. Aumayr and Ms Igenbergs at the Technische Universität Wien in close collaboration with Dr. Schweinzer at the Max Planck Institut für Plasmphysik, Garching-bei-Munchen, Germany. The data will be organised and relayed from Vienna to ADAS in established specific ion data formats with the assistance of ADAS-EU staff. Conversion to charge exchange effective emission coefficients and similar derived data will take place at EFDA-JET Facility and University of Strathclyde. The fundamental and derived data in appropriate ADAS data format collections will be released after assessment and validation to the public domain via OPEN-ADAS [1].

The duration of the project will be twelev months (Jul. 2010 - Jun. 2011) at a fixed price of €10,000.

## 2. Background

The strategy, originated at the JET Facility and now followed by fusion laboratories throughout the world participating in the ADAS Project, for the description of the radiation emission of impurity ions has been the establishment of an integrated atomic data and analysis structure (ADAS). ADAS seeks to provide at appropriate quality, all the derived data required for global modelling and quantitative spectroscopic diagnosis and analysis [2]. The system is based on the initial preparation of collections of fundamental atomic transition probability and excitation rate data for specific ions called *specific ion files*. Various ADAS computer codes then prepare all the derived data such as net power loss coefficients, spectral line contribution functions etc. in a form directly usable in experimental analysis and in plasma models. The fundamental and derived databases are centrally maintained and accessible by standard routines for modelling and diagnostic applications (eg. edge studies, charge exchange spectroscopy and beam emission spectroscopy). Additionally beyond the original scope of ADAS, in EXTENDED-ADAS, codes such as CXSFIT which are more linked to diagnostic analysis are developed and supported by ADAS/ADAS-EU staff in close collaboration with fusion laboratories. In this context there is a specific need to fill a gap in the ADAS beam modelling provision for neutral lithium and sodium beams, used for diagnosis of edge plasma parameter profiles – especially density, but also temperature and impurity concentrations [3]. Continued development and enhancement of neutral beam emission and charge exchange emission diagnostic capabilities are central themes of the ADAS-EU Euratom/Framework 7 Support Action.

The effectiveness and precision in the applications depend on the quality and availability of fundamental data. Recognizing current bounds on computability of certain fusion relevant collision data such as ion impact on neutral targets, ADAS-EU policy falls into two parts. Firstly a modest number of high precision reference calculations and/or measurements at the front edge of current methodologies are sought. These, in their regions of validity, are assessed and combined to provide preferred data which are comprehensive and of extended energy range span. Secondly, as well as

direct embedding of the associated precise data in the databases, the data should be exploited as fiducials which can suggest adjustments or global/regional scalings to the large scale semi-automated mass production calculations of the ADAS baseline. This managed 'lift of the baseline' is a central objective and a primary delivery.

The group at the Institute of Applied Physucs, Technische Universität Wien, originally lead by Prof. H-P. Winter and now by Prof. F. Aumayr has been at the centre of development and implementation of neutral lithium beams as an edge plasma diagnostic [3] in Europe for nearly two decades. They have worked closely in the exploitation and validation of the diagnostic at fusion laboratories including IPP Garching and FZ-Juelich. Also they have given careful attention to procurement of necessary fundamental atomic data for the diagnostics including preparation of key data collections for lithium [4] and sodium [5]. Diagnostic analysis codes for both the lithium and sodium beams were developed at Technische Universität Wien. These codes are now in a frozen state with new code development exploiting Bayesian methods underway at IPP Garching under the guidance of Dr J. Schweinzer [6]. The original codes, with suitable interfacing within IDL-ADAS can fulfil the pedagogical and validation needs for ADAS. In recent years, the Technische Universität Wien group, in close association with Dr J. Schweinzer, have focussed their attention on in-house calculation of key ion impact cross-section data for neutral beams. These calculations are based on the 'close-coupled atomic orbital method'. This, potentially high precision method is particularly suited to the energy region ~50keV/amu typical of current neutral hydrogen heating beams and complements the classical trajectory Monte Carlo and close coupled molecular orbital methods valid at higher and lower energies respectively. The group is extending the scope of CCAO to handle the very many levels sets required by colliders such as $Ar^{+18}$ [7]. Completed calculations include $Be^{+4}$ + H(n=1, 2) [8] and $N^{+7}$ + H(n=1, 2) [9].

ADAS used collisional-radiative modelling, operating on collections of fundamental data, to convert them into the derived data used for plasma models and plasma diagnostic analysis. The collisional-radiative modelling for beam driven charge exchange and beam emission spectroscopic analysis is elaborate. Charge exchange spectroscopy of highly charged species such as $Ar^{+18}$ require nl-resolved and n-resolved models to very high n-shells to describe adequately the redistribution, cascade and re-ionisation leading to the effective emission in useful (normally visible-range) spectrum lines. Also, current models, to allow detailed analysis of neutral hydrogen beam emission, must operate in field disturbed (Stark/Paschen-Back) manifolds with oriented collisions and polarised directional emission. One key to enhanced precision in such models is state selective ion impact excitation and charge transfer by highly charged ions as described above. ADAS machinery allows rapid exploitation of such enhancements to the benefit of the fusion community. In the spatial and temporal non-equilibrium domains, usual ADAS practice (focussed on hydrogen and helium beams) separates metastable and excited populations [10]. The iterative forward modelling with unrelaxed excited states, tied to experimental measurement, as used by Technische Universität Wien, is complementary to the ADAS use. On the other hand, ADAS very high n-shell methods complement Technische Universität Wien collisional-radiative modelling.

This sub-contract provides an opportunity, through guided mapping of data across databases, to extend the scope and lift the quality of ADAS charge exchange and beam emission spectroscopy modelling. The development will have strong synergy with ADAS and other ADAS-EU sub-contracts (cf. Madrid and Groningen) concerned with fundamental ion-atom collision data improvement. It will ensure the preparedness and completeness of ADAS/ADAS-EU for ITER.

**3. The proposed work**

The work falls into four parts, namely database extension for lithium and sodium beams, pedagogical diagnostic model implementation, reference charge exchange/target excitation ion impact cross-sections and assembly of preferred data.

(1) Entry and verification of Technische Universität Wien databases for inelastic collisions of lithium and sodium atoms with electrons, protons and multiply charged ions into ADAS data format adf01 and adf02 (revised).

(2) Assisting ADAS-EU staff in preparation of the Technische Universität Wien/MPI Garching forward modelling lithium/sodium beam density profile determining code and sample data as an ADAS series 3 implementation, with IDL graphical user interface.

(3) Preparation of CCAO state selective charge exchange cross-sections and associated state selective charge exchange cross-sections in ADAS adf01 and adf02 (revised) format for available colliders – to include $Be^{+4}$ and $N^{+7}$ ($Ar^{+18}$ to be included if extended calculations, currently underway, reach suitable completion).

(4) Establishment of preferred adf01 and adf02 (revised) data as above, in agreement with ADAS-EU staff.

Integration of data into ADAS will be executed by staff of ADAS-EU, including the conversion to the key derived data formats, adf12, adf21 and adf22. ADAS-EU staff will pay working visits to Technische Universität Wien to assist with execution of the above tasks as appropriate. A copy of ADAS software will be made available on a workstation at the Institute of Applied Physics, Technische Universität Wien at no charge for local use.

**4. The Financial Provision**

The operations and calculations outlined in the previous section will be carried out over a period of twelve months (Jul. 2010 - Jun. 2011). Financial provision is made as a contribution to the time allocated to the investigation by the senior investigator (Prof. Aumayr) and his research staff. No travel funds or computation costs are sought.

| Item | € |
|---|---|
| Technische Universität Wien (fixed price) | 10,000 |
| total | 10,000 |

**References**


[1] http://www.open.adas.ac.uk
[2] http://www.adas.ac.uk
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# ADAS-EU Travel Report

*Location:* Institute for Theoretical Physics and Astrophysics , University of Vilnius, Vilnius, Lithuania.
*Date:* 31 Mar – 1 Apr 2010.
*ADAS-EU staff:* Hugh Summers.
*Persons visited:* Professor Kupliauskiene, Professor Bogdanovitch, Dr Rancova, Dr Jonauskas, Dr Kucas (Professor Karazija was in-disposed), Dr Kiselius, Professor Rudzikas, Professor Gaigalas.

*Items:*

(1) Discussion centred on establishing an ADAS-EU subcontract with ITPA, University of Vilnius. This would be to place relevant atomic structure and electron impact excitation and ionisation cross-section data for complex atoms and ions into ADAS in support of atomic models and diagnostic spectroscopy of magnetic confinement fusion plasmas.

(2) The Department of Theory of the Atom of the ITPA, itself divides into sub-groups who function largely independently although there is quite substantial overlap in their spheres of interest and in the theoretical methods which they use. Discussions were held with each group separately.

(3) Dr. Kupliauskiene is currently working with a Ukranian experimental group on excitation of autoionising states of Cs in comparison with observed ejected electron features. Single ionization is dominated by the excitation/autoionisation pathway in Cs and in this respect is different from Na. Calculations are made of the resonant states and their decay paths. There appears to be no connection of this work with the role of Cs in $H^-$ beam sources for neutral beams in fusion. Dr Kupliaskiene retains her interest in polarization, that is in spin oriented electrons impacting oriented targets and then the direction and polarisation of emitted radiation and/or particles. The development of the general solution of the angular algebra using the Jucys graphical approach was her major work in 2001/2002. At this stage, utilization of such capability within an ADAS-EU/ADAS framework is not envisaged although it may be helpful for elaborated beam emission studies in the future.

(4) Discussion with Professor Bogdanovitch and Dr Rancova focussed on their modified radial orbital (RO) approach combined with the very large multi-configuation approach of Jucys to represent the CI, including many higher shells (so-called virtual excitations in their parlance). This is an ab initio method without, for example, the radial integral adjustments of Cowan. With heavy complex systems, such as WII and highly charged systems, they find that relativistic effects need to be included in the orbitals leading to quasi-relativisitic transformed radial orbitals (TROs). It is this approach which they have developed and applied in the last two years. Where comparison is possible (the experimental work of Biemont on WII is one point of comparison, but CIV3, MCHF and GRASP are also examined), the present work is rather impressive. They do expand substantially the manifolds of levels for WII. Also for highly charged boron-like isoelectronic sequence members and also for magnesium-like (XeXLIII) comparisons are satisfactory – generally and improvement. This does appear to be a methodology and scope of calculation relevant to fusion and ADAS-EU. Professor Bogdanovitch only deals with structure and transition probabilities. For connection with ADAS adf04, at minimum plane-wave Born collisional rate coefficients would also be required. Bogdanovitch is unfamiliar and uncertain with this step and the group would probably need assistance in its implementation. This seems a small step and would make their work immediately usable and of considerable benefit to ADAS-EU. Dr Rancora would probably be the main implementer although she is now part-time with ITPA.

(5) Professor Karazija was in-disposed so discussions were held with Dr Jonauskas and Dr Kucas of his group. As previously identified, they carry out detailed studies of the Auger/cascade paths following inner shell (photo) ionization. This includes successive electron loss so that the pathways to multiple ionization, as well as single ionization, are described. The pathways examined apply also to electron impact collisional ionization with the photo-ionisation replaced by a direct collisional ionization. Their recent work includes multiple simultaneous electron loss through modelling the relaxation of orbitals in shake-off. Their studies on tungsten ions, from around $W^{+5}$ to $W^{+10}$ indicate the two electron ionization cross-sections as typically <~ 10% of the single ionization cross-section. This is just about large enough to be a relevant correction for dynamic ionization state

modelling and so relevant to fusion and ADAS-EU. It bears on the ADAS-EU subcontract with Mueller.

(6) Professor Karazija and his group study also the key configuration interactions which influence complex atom structure especially through their so-called symmetric exchange of symmetry. This type of CI in the $4p^5 4d^{N+1}$ + $4p^6 4d^{N-1} 4f$ case is found to modify the spectra of ions $W^{+29}$ - $W^{+37}$ weakening some of the lines and strengthening others so that the lines form a much narrower spread group. This is an interesting effect for spectroscopic observation. It is probably present also at the equivalent n=5 shell. Such studies should influence promotion rules used in ADAS baseline modelling for heavy species. This looks like a promising area for ADAS-EU collaboration with Vilnius.

(7) Finally discussions were held with Professor Rudzikas and Professor Gaigalas. I was not up to this point familiar with Professor Gaigalas work. He works with very large scale multi-configuration Hartree-Fock and Dirac-Fock calculations of fine structure, tackling very difficult cases such as transuranic elements $Cm^{+4}$ and $Am^{+3}$. He has written the spin-coupling code for Dirac-Fock (?) implementations and has implemented corrections to Cowan for 4f states (fractional parentage?). Gaigalas work merits further study with a view to inclusion in an ADAS-EU sub-contract.

(8) Generally enthusiasm was expressed by ITPA in sub-contract work for ADAS-EU, although Rancora expressed anxieties about the premier publication demands made on them at Vilnius University. She worried that ADAS-EU type work might distract from this – even though (real) support of fusion is part of their remit as an Associated Laboratory and she certainly found the application area interesting and motivating. Professor Summers will engage to prepare a draft scientific annex for an ADAS-EU sub-contract as soon as possible for further discussion.

HPS
6 April 2010

# ADAS-EU CONTRACT

ATOMIC STRUCTURE AND ELECTRON DATA FOR HEAVY ELEMENT IONS

(1) CONFIGURATION INTERACTION AND RELATIVISITIC/QUASI-RELATIVISTIC STRUCTURE.
(2) AUGER/CASCADE, MULTIPLE IONISATION AND SHAKE-OFF.

H. P. Summers

5 July 2010

## 1. Summary

It is proposed to contract with Prof Alicija Kupliauskiene, acting for the Department of the Theory of the Atom, Institute for Theoretical Physics and Astrophysics, University of Vilnius, Vilnius, Lithuania, to provide a set of calculations of atomic structure together with associated reaction quantities and prescriptions. The reference quality data and studies will establish characteristics of homologous and iso-electronic systems of fourth, fifth and sixth long period elements at low and medium charge states. They will include specification of key configuration interactions and elucidate precision in *ab initio* quasi-relativistic and relativistic calculations. These patterns and the selected specific data will benchmark iso-nuclear and iso-electronic sequence data available in the baseline ADAS database and guide adjustments for further large scale production. The studies will include evaluation of Auger/cascade and shake-off pathways leading to multiple electron - sequential and simultaneous - loss. The latter will be targetted on a selection of heavy species, including tungsten, in moderate states of ionisation ( z ~ 5 - 15) to predict corrections to simple stage-to-stage ionisation in the divertor environment of fusion devices.

The work will make extensive use of the methods and codes developed by Prof. Bogdanovich, Prof. Karazija, Prof. Gaigalas, Prof. Rudzikas and co-workers. The calculations will be performed at the Institute for Theoretical Physics and Astrophysics, University of Vilnius, Vilnius. The data will be organised and relayed from Vilnius to ADAS in established specific ion data formats with the assistance of ADAS-EU staff. Conversion to spectrum line photon efficiencies and similar derived data will take place at the EFDA-JET Facility and University of Strathclyde. The fundamental and derived data in appropriate ADAS data format collections will be released after assessment and validation to the public domain via OPEN-ADAS [1].

The duration of the project will be eighteen months (Aug. 2010 – Jan. 2012) at a fixed price of €10,000.

## 2. Background

The strategy, originated at the JET Facility and now followed by fusion laboratories throughout the world participating in the ADAS Project, for the description of the radiation emission of impurity ions has been the establishment of an integrated atomic data and analysis structure (ADAS). ADAS seeks to provide at appropriate quality, all the derived data required for global modelling and quantitative spectroscopic diagnosis and analysis [2]. The system is based on the initial preparation of collections of fundamental atomic transition probability and excitation rate data for specific ions called *specific ion files*. Various ADAS computer codes then prepare all the derived data such as net power loss coefficients, spectral line contribution functions etc. in a form directly usable in experimental analysis and in plasma models. The fundamental and derived databases are centrally maintained and accessible by standard routines for modelling and diagnostic applications (eg. edge studies, VUV and XUV spectroscopy). The effectiveness and precision in the applications depends on the quality and availability of fundamental data. In this context a specific need is enhanced provision for low and medium ionisation stages of heavy elements up to and including tungsten. Such enhancement is a central theme of the ADAS-EU Euratom/Framework 7 Support Action. Recognizing the complexity of some of the fusion relevant heavy element ions and current bounds on atomic reaction computability, ADAS-EU policy falls into two parts. Firstly a modest number of high precision reference calculations and/or measurements at the front edge of current capability are sought. Secondly, as well as direct embedding of the associated precise data in the databases, the data should be exploited as fiducials which can suggest adjustments or global/regional scalings to the large scale

semi-automated mass production calculations of the ADAS heavy element baseline. This 'lift of the baseline' is the central objective and the primary delivery.

The Department of the Theory of the Atom at the Institute for Theoretical Physics and Astrophysics, has a long history of research in complex atomic structure, very large multi-configuration approaches and efficient algebraic methods, stemming from the original work of Prof. Yutsis on through the work of Prof. Rudzikas through to the present day and the work of Profs. Kupliauskiene, Karazijas, Bodganovich and Gaigalas. Their associated research groups exploit these broad methods in specific unique areas which can be of special value to the magnetic confinement fusion program as it seeks to model, analyse and exploit heavy species such as tungsten for ITER. Thus the modified radial orbital (RO) approach combined with the very large multi-configuration approach with 'virtual excitations' of Prof. Bogdanovich and Dr Rancora, extended to quasi-relativistic transformed radial orbitals (TROs) [3, 4], allows *ab initio* access to systems as complex as WII with good precision. The team of Prof. Karazijas evaluates 'global characteristics' [5] which rank the key configuration interactions, such as 'symmetric exchange of symmetry' influencing accurate theoretical atomic structure [6]. These effects can constrain the spread and relative intensities of individual components of very large transition arrays. This team has special expertise in Auger/cascade, shake-down and shake-off, originally applied to photoionisation [7], but more recently to multiple electron loss in electron impact ionisation of low ionisation stages of tungsten. The group of Prof. Gaigalas works with very large scale multi-configuration Hartree-Fock and Dirac-Fock calculations of fine structure, tackling very difficult cases such as transuranic elements [8]. The group has special interests in efficient coding of spin algebra for Dirac-Fock codes and the correct handling of f-states.

These advanced theoretical capabilities connect well with the layered precision approach of ADAS and ADAS-EU for bringing all relevant heavy elements into effective modelling and analysis for ITER. Of principal concern is modelling and diagnostic spectroscopy of heavy elements within the divertor and scape-off-layer, which spans charges states from neutral to < 20. The baseline ADAS database for ionisation state, excited population state, radiated power and emissivities centres on automatic creation of configuration sets for each ion, optimised on contributors to total radiated power. This approach, suited to superstaging and general 2-D divertor modelling, should be selectively improved for specific radiators and in particular specific homologous systems and iso-electronic sequences dictated by spectroscopy. The configuration selection prescriptions, evaluated for heavy element ions of the Department of the Theory of the Atom can directly modify/extend the promotional rule sets of the ADAS baseline. Secondly the explicit atomic structure and transition probability outputs for selected ions from the Department of the Theory of the Atom may be routed through the ADAS processing steps to specific ion datasets of fundamental ADAS data format adf04. At this point, automatic passage through ADAS derivative processing is enabled, lifting the baseline systematically. It is this chain of exploitation, suitably supported by close engagement for ADAS-EU staff with researchers of the Department of the Theory of the Atom, which the sub-contract in broad terms intends to achieve.

This sub-contract is concerned with using theoretical methods to lift the quality of the ADAS databases. It links to other sub-contracts providing experimental measures of energies, transition probabilities, ionisation cross-sections and recombination rate coefficients. Collectively these benchmarking studies on reference elements and ion will guide parametric adjustments globally to ADAS derived data. The enhanced theoretical relativistic and quasi-relativistic structures of the targetted systems will provide in turn the stepping-off point for the highest grade electron impact collision cross-section calculations in due course and completion of the heavy element theme of ADAS-EU.

**3. The proposed work**

The work falls into four parts, *ab initio* structure and transition probability calculations in the large scale multi-configurational approach with virtual excitations and TROs, global characteristics and CI prescriptions, Auger/cascade pathways and multiple ionisation, selected Dirac-Fock calculations for neutral/near neutral very heavy systems.

(1) Multiple electron ionisation rate coefficients, with special emphasis on 4d, 4f and 5d, 5f open shell systems. The study should be based on contiguous sets of iso-nuclear ions of selected elements from which approximate general prescriptions can be inferred. This will include design of an extension of ADAS data formats adf23 and adf07.

(2) Exploitation of ITPA special studies of key complex ion configuration interactions (such as symmetric exchanger of symmetry), by inclusion in ADAS data format adf54, tuned to primary resonance line spectroscopy, with special emphasis on 4d, 4f and 5d, 5f open shell systems..

(3) A benchmark study for WI, WII, and WIII using the Bogdanovich quasi-relativisitic (TRO) approach. The structure and transition probability study will be extended to implement plane wave Born cross-sections so that delivery can be in the form of ADAS adf04 datasets. Professor Nigel Badnell for ADAS-EU will collaborate with Professor Bogdanovitch and his co-workers and provide support procedures and sub-routines so that the link from structure to plane-wave Born can be made.

(4) A benchmark study in Dirac-Fock approximation of a selected lanthanide-like ion in a low charge state ( ~6-12). The study is designed to assess the possibility of more extensive use of such heavy elements as markers (observed in low ionisation stages in divertor regimes) and edge transport studies and cross-reference other approximate studies of low charge state tungsten ions. Suitable ions would be $W^{+8}$ (Dy-like) or $Au^{+8}$ ( Yb-like).

Integration of data into the ADAS system will be executed by staff of ADAS-EU. ADAS-EU staff will engage closely with ITPA in the study, assisting in the passage of the general prescriptions and results into the ADAS data formats [9], especially adf04, adf07, adf23 and adf54. ADAS-EU staff will pay working visits to University of Vilnius to assist with execution of the above tasks as appropriate. A copy of ADAS software will be made available on a workstation at the Department of Physics, University of Vilnius at no charge for local use.

**4. The Financial Provision**

The operations and calculations outlined in the previous section will be carried out over a period of eighteen months (Jul. 2010 - Dec. 2011). Financial provision is made as a contribution to the time allocated to the investigation by the senior investigators (Prof. Bogdanovich, Prof. Karazija, Prof. Gaigalas) and their research staff. No travel funds or computation costs are sought.

| Item | € |
|---|---|
| University of Vilnius (fixed price) | 10,000 |
| total | 10,000 |

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# ADAS-EU Travel Report

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| *Location:* | Centre for Theoretical Atomic, Molecular and Optical Physics , Queen's University, Belfast. |
| *Date:* | 25 Mar 2010. |
| *ADAS-EU staff:* | Hugh Summers. |
| *Persons visited:* | Dr Penny Scott, Dr Cathy Ramsbottom, Dr Patrick Norrington (Professor Burke was indisposed and was unable to be present). |

*Items:*

(1) Discussion centred on establishing an ADAS-EU subcontract with Queen's University, Belfast. This would be to place relevant atomic structure and electron impact cross-section data for complex atoms and ions into ADAS in support of atomic models and diagnostic spectroscopy of magnetic confinement fusion plasmas.

(2) Professor Summers explained the key zones of concern for increased precision and coverage of atomic data - both in preparation for ITER and for the on-going programmes of current fusion machines in Europe, including the JET Facility after the EP2 upgrade. He explained the increased importance of heavy species, especially tungsten for ITER, AUG and JET EP2 and the efforts being made to fit such species into 2-D impurity transport models. He also explained the need to observe and interpret such species as inflowing neutrals from sputtering surfaces, to obtain spectral measurables in the divertor region in-spite of spectral complexity and the special role of few valence (closed shell or one or two electrons outside closed shells) electron isoelectronic systems for the most effective analysis. Professor Summers emphasized the importance of a layered approach of different precision and completeness to the whole scope of atomic data for heavy atoms and the potential role of Queen's in reference/benchmark calculations which could adjust and characterize the precision of simpler calculations.

(3) Initial discussion of Belfast codes and capabilities centred on the atomic structure and transition probability efforts led by Professor Hibbert. The recent publication on neutral tin (J. Phys.B. (2008)41, 165003), partly motivated by the MAST studies of Foster, illustrated the potential of very large CIV3 calculations. A similar pathway through correcting, correlation and polarization orbitals would probably be required for WI. It was felt that Professor Hibbert, although absent on holiday, would be prepared to devote some of his expertise to an ADAS-EU sub-contract in this area.

(4) It was noted that the above SnI data is not entered in ADAS. Professor Summers pointed out that the ADAS adf04 format input datasets for population modelling require collisional rates as well as structure and A-value data. He also stressed that the latter data, even in plane wave Born approximation - provided the structure is good - are valuable for fusion. Such Born approximation is a simple step of Bessel matrix element evaluation once the bound state wave functions have been established and is a key part of an automatic communication path to ADAS.

(5) Professor Summers drew attention to the ADAS-EU sub-contract activity with Professor Biemont and co-workers at University Mons-Hainaut on wavelength and life-time measurements for complex systems such as lanthanides and WII which would link well to Belfast CIV3 benchmark calculations.

(6) Discussion turned to R-matrix calculations of electron impact cross-sections. The Belfast staff clarified and contrasted the varying approaches. Within the broad Breit-Pauli framework, the lead Queen's development is PRMAT, a sophisticated parallel implementation, based in the inner region on RMATRX2/95, in which the intermediate coupling transformation is made at the R-matrix inner region boundary. The outer and asymptotic regions are then handled by the PFARM parallel code. Considerable efforts have been made and continue to optimize and future proof the parallelism. In particular for supercomputers such as the HECTOR Phase 1 Cray XT4, efficient allocation of sectors, assignment of more than one process to each sector and so on are required to bypass current bottlenecks. It is noted that on-going work on PRMAT at Daresbury relies on Dr Noble, who though now retired is continuing development work. It appears that PRMAT, within these limitations is functional and capable of very large calculations of the sort envisaged for heavy species for fusion.

(7) The alternative for Breit-Pauli R-matrix is the parallelization by Ballance, using a parallelized STGF and the Badnell ICFT transformation to intermediate coupling in the asymptotic region. The Queen's group also uses this method and does not express a strong

preference for either. One surmises that setting up PRMAT optimally for complex systems requires effort and experience which is still evolving.

(8) In the fully relativistic domain GRASP (variants) and DARC provide the structure and R-matrix collisional capability. Dr. Norrington is an developer of both with Dr Grant, but new development such as Dirac R-matrix with pseudostates (DRMPS) and parallisation is shared between Dr. Norrington and other co-workers of Professor Badnell at University of Strathclyde. PRMAT is uniquely a Queen's development.

(9) Much of the Queen's production is linked to astrophysics. In particular, they have put substantial effort into iron-peak elements and their ions such as FeII and FeIII. The number of levels and spectrum lines of such ions is very large and expanding with each calculation. From a fusion point of view, it is more likely to be diagnostically fruitful – in the sense of fewer identifiable lines – to work with isoelectronic systems with closer to fully filled active shells, such as nickel-like (3d10) or similar systems in the fifth and sixth periods. The Queen's team expressed interest in calculating iso-electronic members of such systems with a view to using such benchmarks to make scaling/adjustments to cruder data currently making up the ADAS baseline.

(10) Returning to the neutral and near-neutral complex systems, The Belfast group pointed out the necessity to reduce the number of basis states in the Hibbert structure expansion before R-matrix collision calculations are possible – a task familiar to them. Dr. Norrington also expressed the view that he would interested to address the heavy neutrals (such as WI) with GRASP/DARC directly.

(11) Generally enthusiasm was expressed by the Queen's group in sub-contract work for ADAS-EU. It appeared that the permanent staff who participated in our discussions would themselves see to the implementation of agreed ADAS-EU calculations. Professor Summers will engage to prepare a draft scientific annex for an ADAS-EU sub-contract as soon as possible for further discussion.

HPS
6 April 2010