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OPEN-ADAS report 1

24 June 2010

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OPEN-ADAS report 1

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Abstract: *The report reviews OPEN-ADAS activities for project months 1-18*

Contents

Preface

The report is one of a series of four such reports, deliverable under the ADAS-EU project, which assemble documentary material of OPEN-ADAS for the applicable year. Each comprises a summary of OPEN-ADAS user activity, developments and release notes.

H P Summers
24 June 2010

Chapter 1

Overview

OPEN-ADAS is the name of the path for release of ADAS data and support software into the public domain. It is an agreed and shared project between ADAS and the International Atomic Energy Agency, Atomic and Molecular Data Unit, Nuclear Data Section (IAEA) in Vienna. As agreed in the ADAS-EU proposal, OPEN-ADAS is to be used for public domain release of fundamental and derived atomic data which enters the ADAS databases from ADAS-EU activities.

The primary OPEN-ADAS software preparation, beta testing and release were achieved according to plan late in 2008 before the commencement of ADAS-EU. The web server is located at the Physics Department, University of Strathclyde and linked to IAEA Vienna. The OPEN-ADAS Version 1 release document and manual is attached in Appendix A [1]. The web address is *www.open.adas.ac.uk*.

The OPEN-ADAS development has continued through 2009 with addition of the freeform search capability, extension of the released ADAS data formats and extension of the downloadable software for its utilisation in users' own codes. An OPEN-ADAS update report was prepared as a presentation for the annual Data Centre Network (DCN) coordination meeting at IAEA in Sep. 2009. The report is attached in Appendix A [2]. It has been agreed that ADAS should formally become a member of the IAEA DCN in an on-going relationship which will help to ensure the continuation of OPEN-ADAS.

The present ADAS-EU report 'OPEN_1 was scheduled for month 11. It is convenient to bring this document up-to-date as at month 18. The next substantive update to available data through OPEN-ADAS will take place around August 2010 and will be reported in 'OPEN_2' towards the end of the year.

Dr Allan Whiteford was the developer of the OPEN-ADAS software. His departure from the University leaves a personnel gap for OPEN-ADAS maintenance. Dr Martin O'Mullane has taken over this role and now acts as the communication path with IAEA and the DCN. Since the primary software of OPEN-ADAS is in place, further data release is the main issue for ADAS-EU, so no major problem is anticipated in Dr O'Mullane's fulfillment of this role.

As at 24 June 2010, OPEN-ADAS is proving a very effective and well used public domain path to ADAS data. There are two hundred and six registered users from thirty-five countries spanning all continents. Eleven distinct ADAS format have been accessed which cover all the themes of ADAS-EU. There have been three thousand seven hundred and five data set viewings and one thousand seven hundred and sixty eight downloads.

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Chapter 2

Work package reports

2.1 Work package 26-2-1

The work package task comprises the preparation of this report

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Appendix A

OPEN-ADAS documents and updates

[1] OPEN-ADAS: Version 1
[2] OPEN-ADAS: Update 2009

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OPEN-ADAS Version 1.0
Final Report

`http://open.adas.ac.uk`

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August 2008

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This work was financed jointly by the IAEA and the ADAS Project.

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Abstract

The present report describes version 1.0 of the OPEN-ADAS system as released in July 2008.

OPEN-ADAS is a system to search and disseminate key data from the Atomic Data and Analysis Structure (ADAS) over the web. The primary objective of ADAS is support of the magnetic confinement fusion programme and the on-going development of ADAS is enabled by the ADAS Project and its membership. The OPEN-ADAS development has therefore a dual benefit, namely to enable non-members, with an interest in fusion, to download and use[1] ADAS data, and also to provide ADAS Project members with a more intuitive searching mechanism for ADAS data.

Section 1 gives the background to the OPEN-ADAS system and section 2 gives precise details of the scope of OPEN-ADAS and the data which is released with the system. The design and implementation of the indexing system are discussed in section 3. The web interface to OPEN-ADAS is presented in section 4 with details given as to its general use. Attention is given to the various searching mechanisms. Software and documentation have also been released with OPEN-ADAS. These are discussed in section 5.

The appendices to this report provide extended information on the specific implementation. Appendices D, E and F give details of the extensive OPEN-ADAS beta-testing process.

[1]Subject to terms and conditions — see appendix G.

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Acknowledgments

Acknowledgment for this work is given to the JET Joint Undertaking[2] for originally developing ADAS. The continued support of the ADAS Project members is also acknowledged. The ADAS database itself includes data from a very large number of contributors, too numerous to mention here.

Funding for the development and implementation of OPEN-ADAS was shared equally by the IAEA and the ADAS Project itself. The University of Strathclyde has managed the development and provided the computational facilities and specialist expertise for its execution.

The work would not have been possible without the availability of a large number of open-source projects including, but certainly not limited to, Linux, Apache, MySQL, PHP, Perl and many pieces of software developed and provided by the Free Software Foundation.

Finally, the OPEN-ADAS beta testers are gratefully acknowledged. Their time is greatly appreciated and their feedback was of great value. They are: Nigel Badnell, Kurt Behringer, Mathias Brix, Paul Bryans, Bob Clark, Rémy Guirlet, Denis Humbert, Ratko Janev, Stuart Loch, Chris Nicholas, Thomas Pütterich, Randall Smith and Mike Witthoeft.

[2]The JET Joint Undertaking was reconstituted in 2000 as the EFDA-JET Facility with the UKAEA, Culham Laboratory as the operations manager. EFDA-JET and UKAEA have continued the JET support of ADAS.

1 Introduction

OPEN-ADAS is a system to search and disseminate key data from the Atomic Data and Analysis Structure (ADAS)[3] over the web. The extensive high quality fundamental and derived atomic data for fusion in the ADAS databases generated by ADAS, by the ADAS Project and by its many associates are a major resource. It is beneficial for this to be in the public domain, independent of ADAS Project membership, as a guided provision. This provision is the main thrust of OPEN-ADAS. Other aspects which support this primary objective include improved documentation and the supply of subroutines for reading the data.

There is also a need from within the ADAS community to provide better guidance on selection of the most suitable ADAS data for specific applications. OPEN-ADAS fulfills a large part of this need by allowing a number of flexible searching mechanisms of the ADAS database.

The data contained within ADAS is strictly organised and precisely formatted. There are forty-nine distinct types of data file and ADAS at this time contains 19,572 data files with a total size of 2.8GB.

Many of the files contained within ADAS are so-called 'driver files' for other ADAS codes and are thus unsuitable and inappropriate to circulate via OPEN-ADAS. Others are tuned to particular applications and are also of lesser general interest. We note that the interactive ADAS programs and callable subroutines consist of just under one million lines of source code. The scope of OPEN-ADAS is targetted on and limited to the release and organisation of general user relevant data from the ADAS databases and the provision of code, subroutines and procedures to enable such users of OPEN-ADAS to read the released data (see section 5).

A schematic of the overall OPEN-ADAS system is shown in figure 1. The system operates by parsing each of the ADAS files and creating a tag file (see section 3.1 for details). These tag files are then inserted into a relational database (see section 3.2) and is browsed using a web interface (see section 4) which also allows downloading of data.

[3]The Atomic Data and Analysis Structure (ADAS) is a computer program and data package developed at JET Joint Undertaking to assist in analysis of spectral radiation and in modelling radiating properties of plasmas. In the period 1994-1996 a plan was devised and enacted, called the ADAS Project, for a complete conversion of JET-ADAS to workstations. Managed by the University of Strathclyde, this provided a regulated path on dissemination approved by JET Joint Undertaking so that ADAS was available to relevant participating laboratories. Since 1996, with the approval and funding support of participants, ADAS has continued in on-going maintenance and extended development. Participation in the project has increased with most large fusion laboratories in the world now members.

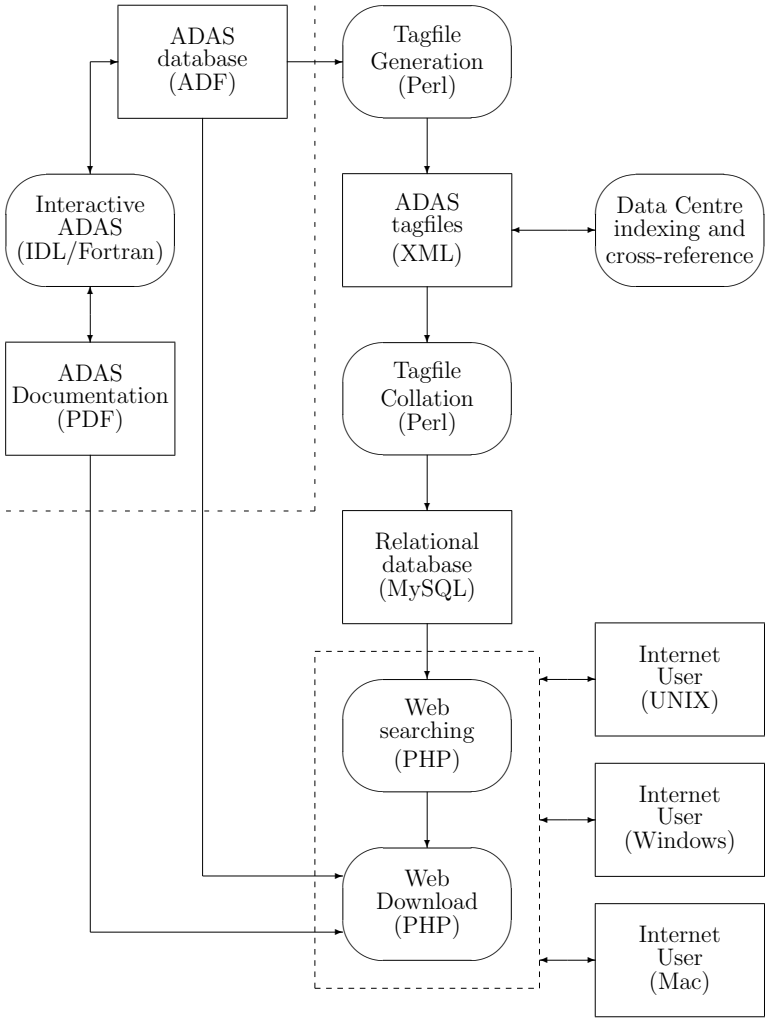

Figure 1: Schematic of the OPEN-ADAS system with specific programming languages and data formats displayed in brackets. The area in the upper left represents the interactive ADAS system (IDL-ADAS) available to ADAS Project members. The area at the bottom represents a web server handling simultaneous requests from multiple browsers and operating systems.

2 OPEN-ADAS data

ADAS data files are ASCII character files. They divide into forty-nine different types each with its own application-specific internal formatting These formatting specifications are numbered and called ADAS Data Formats ('ADF' for short), comprising ADF00 to ADF48. Table 1 outlines the data formats for initial release with OPEN-ADAS. All are primarily fusion-oriented. We note that the version of the full ADAS system/database associated with version 1.0 of OPEN-ADAS is ADAS v2.13.

Format	Description	Files	Size
	Fundamental data		
ADF01	Charge exchange Cross sections	118	1.9 MB
ADF04	Resolved specific ion data collections	1132	463.8 MB
ADF07	Electron impact ionisation coefficients	67	589.4 kB
ADF08	Radiative recombination coefficients	100	465.4 kB
ADF09	Dielectronic recombination coefficients	1619	1.1 GB
	Derived data		
ADF11	Iso-nuclear master files	352	45.4 MB
ADF12	Charge exchange emission coefficients	43	1.1 MB
ADF13	Ionisation per photon coefficients	153	35.2 MB
ADF15	Photon emissivity coefficients	176	74.5 MB
ADF21	Effective beam stopping coefficients	218	1.8 MB
ADF22	Effective beam emission coefficients	402	3.4 MB
	Total	4228	1.58 GB

Table 1: Data formats released with OPEN-ADAS along with the total number of distinct files in each format and the total size of the files. See text for details of the distinction between *fundamental* and *derived* data.

For analysis of the emission and transport of impurity species in a fusion plasma there exist a number of useful atomic deliverables. These quantities can be applied directly to spectroscopic measurements or be fed into models without unnecessary complications. It has been the trend in atomic data centres (e.g. IAEA[4] and NIFS[5]) to collect, archive and validate fundamental data such as wavelengths, transition probabilities and single reaction cross-sections. While cross-sections are appropriate quantities to collate and compare, they are not immediately useful to a fusion plasma diagnostician studying trace impurity species or to transport modelling codes. Rather the

[4] `http://www-amdis.iaea.org/`
[5] `http://dbshino.nifs.ac.jp/`

fusion need is for quantities such as photon emissivity coefficients, photon efficiencies, total effective ionisation/recombination rates and radiated power coefficients. These are derived quantities, usually the resultant of many reactions and depending on local plasma conditions of temperature and density. They are calculated with atomic population modelling (called collisional–radiative) codes. The code output values, that is the derived quantities, are tuned to the diagnostician's or modeller's needs and the user may require only passing knowledge of the fundamental underpinnings.

The ADAS database makes this distinction between fundamental and derived data and OPEN-ADAS puts particular emphasis on the dissemination of such application-relevant derived data; in this sense it is unlike the majority of atomic databases. The data released with OPEN-ADAS is complementary to other web-based atomic databases in that it does not seek to catalogue and collect fundamental cross sections as individuals, but deals with comprehensive collections of such data which allow the derivative calculations. Of course, the fundamental data release with OPEN-ADAS is also a major resource but we note that much of it was largely in the public domain before the release of OPEN-ADAS.

For application to many aspects of the spectral emission from fusion plasmas, the derived atomic data provided must not only be dependent on temperature and density but also be matched to the dominant populations of species in the plasma as they evolve dynamically in space and time. For fusion plasmas, these dominant populations may be metastable states as well as ground states and so collisional–radiative population modelling should ideally be 'metastable resolved'. This is called generalised collisional–radiative (GCR) modelling. Metastable-resolved emissivity coefficients, effective recombination coefficients and so on described in this work are some of the important and highest quality outputs of OPEN-ADAS (Summers *et al* 2006). The simpler, so called 'stage-to-stage' picture, in which it is assumed that only the ground state of each ionisation stage has a substantial population density in the plasma, gives the more familiar collisional–radiative modelling and coefficients. The latter 'metastable unresolved' data occurs extensively in ADAS since then very complete coverage of elements is possible, albeit at lower quality.

Generally ADAS data files contain as far as possible familiar quantities in familiar units, such as emissivity coefficients (photons cm^3 s^{-1}) — avoiding complicated multiplying factors. Scaling is used when tabular data would be badly conditioned for interpolation and/or lose numerical precision. Also, when data behaviour along iso-electronic sequences is relevant or when ensuring that independent variables of tabulations remain in useful ranges, scaling may be used. The most common is scaled ranges of electron temperature,

T_e, and electron density, N_e with effective ion charge, z, as $T_e/(z+1)^2$ and $N_e/(z+1)^7$. The matching scaling of coefficients are called 'reduced coefficients' in ADAS. ADAS data format specifications must be read carefully to ensure correct interpretation of data file quantities.

2.1 ADAS terminology

The terminology used within ADAS and OPEN-ADAS can sometimes be unfamiliar and lead to confusion. In this section, attention is drawn to a number of terms which may be ambiguous and require clarification.

- **Acronyms and mnemonics**: ADAS uses a number of acronyms and mnemonics for certain data formats and sub-classes. There are also some simple abbreviations. These are quite widely used in the fusion community but may not be generally familiar. They occur in text both as upper and lower case forms. They include:
  - *ADF*: ADAS data format
  - *CXS*: charge exchange spectroscopy, normally beam driven
  - *MSE*: motional Stark effect, affecting beam atom emission
  - *RR*: radiative recombination - ADF08
  - *DR*: dielectronic recombination - ADF09
  - *CR*: collisional–radiative coefficients - ADF11. Subclasses:
    - *ACD*: effective recombination
    - *SCD*: effective ionisation
    - *CCD*: effective charge exchange recombination
    - *PLT*: effective low-level line power
    - *PRB*: effective recom + Brems power
    - *PRC*: effective charge exchange power
  - GCR - generalised collisional–radiative coefficients - ADF11. Subclasses as CR +:
    - *QCD*: effective metastable cross-coupling
    - *XCD*: effective parent metastable cross-coupling
  - *CD*: collisional-dielectronic (synonym for collisional–radiative)
  - *QEF*: effective emission coefficient (from CXS normally) - ADF12
  - *SXB*: ionisation per photon coefficient - ADF13
  - *PEC*: photon emissivity coefficient - ADF15

  - *BMS*: beam stopping coefficient - ADF21
  - *BME*: beam emission coefficient - ADF22

- **Bundling and resolution**: Depending on circumstances, it may not be helpful or possible to deal with the populations of excited states of ions in a plasma at the detail of individual levels. Rather, one deals with the populations of groups of levels, such as of all the levels of a term, of all the levels of an $nl-$shell or of all the levels of an $n-$shell. The collisional–radiative calculations are then referred to as being in a 'bundle-nl' or 'bundle-n' approximation. This bundling is sometimes described as the 'resolution level' of the calculations (and of the consequential derived data. Other relevant resolution levels of ADAS data are 'term' (or 'LS' or 'ls') and 'level' (or 'LSJ' or 'ic'). 'bundle-nl' is also called 'ca'[6]. 'ic' and 'ca' are short for 'intermediate coupling' and 'configuration average' respectively. Resolution in this context is related to but a bit different from 'metastable resolution'.

- **Condensation and projection**: In GCR studies, it is efficient and physically appropriate to couple a lower resolution population model, such as 'bundle-n' for very many highly excited levels, to a high resolution model, such as 'ic' for the set of lowest levels. Then one says that the influence of the bundle-n results for the high levels are condensed or projected onto the low levels. Projection matrix files (ADF17) and mapping files (ADF18) enable this in ADAS.

- **Data formats and ADF numbers** The ADAS 'database' is organised using a collection of ASCII files sitting on a conventional UNIX filesystem. See also table 1. Files are grouped together in directories. At the top level of this database are a set of file-formats called ADAS Data Formats (or ADFs). These formats are all distinct and refer to different types of data (e.g. ADF15 are effective emission coefficients). The ADAS data format name, such as ADF15, is used to refer both to the formatting specification and the name of the top level data set directories.

- **Date conventions**: ADAS filenames often have a two-digit year number embedded in them. These numbers should be treated as a token and do not necessarily reflect when a particular file was introduced. Typically it indicates when a particular approximation or quality level was

[6]Typically, 'bundle-nl' is used when referring to hydrogenic systems (i.e. a single electron or one electron outside a closed core) and 'ca' when referring to more complex systems.

introduced. For example, for GCR data such as ADF11 and ADF15, the year '96' was the year of its substantive introduction into the ADAS database. Information on the actual year a file was produced is available in the comments section of each file.

- **Sub-directory naming conventions**: Sub-directories at one level below the ADAS data format commonly contain files of a particular element (an iso-nuclear set) or files of ions with the same number of electrons (an iso-electronic set). For the former '#<nuclear charge number>' appears as a post-fix of the sub-directory name (such as *copmm#18* for argon). For the latter '#<chemical symbol of first member>' appears as a post-fix of the sub-directory name (such as *pec96#be* for beryllium-like). Although this is present practice, some older ADAS directories are inconsistent.

- **File naming conventions**: Actual data files, as distinct from directories, all have the extension '.dat'. The whole file name, if one of an automatic or semi-automatic production process are typically of the form '<resolution>#<element><ion charge>.dat' such as *ic#ar10.dat*. If hand produced by a specialist, typically author initials appear in the file name. Again there are many older ADAS datasets which do not conform to the present conventions.

- **Derived data**: Derived data are data which have been processed through a collisional–radiative model and have dependency on plasma parameters. These are data like *effective* ionisation/recombination rates (i.e. the driving terms for transport models) and *effective* emission coefficients.

- **Fundamental data**: Fundamental data are data which are specific to an ion in isolation or composed of individual pure reactions. These are things like energy levels, spontaneous radiative rates, state resolved recombination/ionisation rates and collision cross-sections. Maxwell averaged rate coefficients (or reduced forms such as Υ) between specific levels are viewed as fundamental data.

- **J values and statistical weights**: The quantum number assignment of energy levels in ADAS data files such as ADF04 appear as $(2S + 1)L(J)$. There is a long-standing convention in ADAS that the actual meaning of the J field is '(statistical weight-1)/2' independent of the coupling scheme. This is true for level resolved data. For term resolved data we also follow the convention which means that a ^{3}P level would

have an apparent J-value of 4 but it actually gives the correct statistical weight of the term as 9. Consequently ADF04 files of varying bundling can be handled transparently in collisional–radiative modelling.

- **Metastable unresolved**: In a stage-to-stage, metastable unresolved picture, there is often confusion as to whether metastables are included or not in the population structure. They are, but they are treated as thought they were ordinary excited states and therefore assumed in quasi-static balance with the ground state. Also their contribution to the total population, summed over all levels, of the stage (which is usually assumed to be that of the ground population alone to good precision) is omitted, unless special re-normalising steps have been taken in the collisional–radiative calculations. Such information is contained in ADAS data set comments and should be looked out for to avoid misunderstanding.

- **Quasi-static approximation**: Collisional–radiative theory is concerned with the relative relaxation times of different state populations of ions in plasmas. Appropriate separation of those with short (ordinary excited states) and those with long (ground and metastable states) relaxation times takes place according to plasma (mainly density) regime. The valid and simplifying approximation is made that those with short lifetimes can be assumed in statistical equilibrium with the instantaneous values of the long-lived populations. Then the solution of the collisional–radiative equations is easier to obtain, delivers universal derived data which are functions of local plasma conditions only and separates cleanly into the data formats required for establishing ionisation state (in dynamic plasma models) and then subsequent emission.

2.2 ADF01

Bundle-n and bundle-nl charge exchange cross-sections

The data sets provide principally nl-resolved charge exchange cross-sections over a range of n-shells for a donor neutral atom (typically hydrogen) colliding with an ionised impurity receiver as a function of normalised collision energy (keV/amu). The reaction is

$$X^{z+} + H^0_{n'} \rightarrow X^{(z-1)+}_{nl} + H^+ \tag{1}$$

The data include summed cross-sections to whole n-shells and the total cross-section summed over all n-shells. The data may be used for any of the

hydrogen isotopes. Parameters are usually also present which represent the cross-sections at high n-shells outside the tabular range and asymptotically at high collision energy. The energy ranges are suited to neutral beam studies and are generally too high for relevance to thermal charge transfer. The receiving ions are, for the most part, the bare nuclei of light elements up to neon. The donor states of hydrogen include the ground state and may include $n' = 2$ and 3 states. There are a smaller number of data sets in which neutral helium, lithium and sodium are the donors. Normally the data sets are used in collisional–radiative models of the emissivities (including emissivities in the visible wavelength range) of the receiver as driven by the charge exchange. These derived data, which are more suited to spectroscopic interpretation of charge exchange signals, are tabulated in ADF12.

2.3 ADF04

Resolved specific ion data collections

The data sets provide energy levels, and rate coefficient data for the ground and low levels of an ion up to some cut-off shell. The coefficient data includes, at minimum, spontaneous emission coefficients and electron impact collisional rates between the level set sufficient for a collisional–radiative population calculation and emissivity prediction. The electron impact collisional rate coefficients are tabulated as the quantity Υ which is a function of electron temperature (K). Υ is the Maxwell-averaged collision strength and is a preferred quantity for tabulation due to its symmetry between initial and final states and its slow variation with temperature. For the electron impact excitation reaction,

$$X_i^{z+}\left(E_i\right) + e\left(\epsilon_i\right) \rightarrow X_j^{z+}\left(E_j\right) + e\left(\epsilon_j\right), \tag{2}$$

with $\epsilon_i + E_i = \epsilon_j + E_j$, where E_i and E_j are excitation energy energies and E_1=0, the transition energy is $\Delta E_{i,j} = E_j - E_i > 0$. Then with T_e the electron temperature the relationships are:

$$\Upsilon_{ij}\left(T_\mathrm{e}\right) = \int_0^\infty \Omega_{ij}\left(\epsilon_j\right) e^{-\epsilon_j/kT_\mathrm{e}} d\left(\frac{\epsilon_j}{kT_\mathrm{e}}\right). \tag{3}$$

The excitation and de-excitation rate coefficients are

$$q_{i\rightarrow j}\left(T_\mathrm{e}\right) = 2\sqrt{\pi}\alpha c a_0^2 \frac{1}{\omega_i} e^{-\Delta E_{ij}/kT_\mathrm{e}} \left(\frac{I_\mathrm{H}}{kT_\mathrm{e}}\right)^{\frac{1}{2}} \Upsilon_{ij} \tag{4}$$

and

$$q_{j\rightarrow i}\left(T_{\mathrm{e}}\right)=2\sqrt{\pi}\alpha c a_0^2\frac{1}{\omega_j}\left(\frac{I_{\mathrm{H}}}{kT_{\mathrm{e}}}\right)^{\frac{1}{2}}\Upsilon_{ij} \tag{5}$$

α is the fine structure constant, c is the speed of light, I_{H} is the ionisation potential of hydrogen, ω_i is the statistical weight of the lower level, ω_j is the statistical weight of the upper level and a_0 is the Bohr radius. Ω_{ij} is the collision strength related to the excitation and de-excitation cross-sections by

$$\Omega_{ij}\left(\epsilon_j\right)=\omega_i\left(\frac{\epsilon_i}{I_{\mathrm{H}}}\right)\left(\frac{\sigma_{i\rightarrow j}\left(\epsilon_i\right)}{\pi a_0^2}\right)=\omega_j\left(\frac{\epsilon_j}{I_{\mathrm{H}}}\right)\left(\frac{\sigma_{j\rightarrow i}\left(\epsilon_j\right)}{\pi a_0^2}\right). \tag{6}$$

The scope of the collisional–radiative calculation which the data set can support many be enhanced if it includes additional transition data for further processes. Transition lines in the ADF04 data set have a code letter which indicates the transition line type. Table 2 summarises these codes. An ADF04 data set with 'R' and 'S' lines can support a GCR population model and, with 'H' lines, one which includes neutral hydrogen charge exchange driven recombination and emission. Users of ADF04 data sets should examine the comments section to see what is included. Sub-directories of the ADF04 format typical contain groups of files with similar capability covering iso-nuclear or iso-electronic sequences. There are very many ADF04 files and the appropriate one for a particular purpose should be chosen carefully. Note that ADF04 is a fundamental data format. It is the data formats ADF11, ADF13 and ADF15 produced after collisional–radiative calculations using an ADF04 data set which are most relevant to application.

Code	Meaning
' '	unspecified electron impact excitation data
'1'	dipole electron impact excitation data
'2'	non-dipole, non-spin change electron impact excitation data
'3'	spin change electron impact excitation data
'P'	positive ion impact excitation data
'R'	free electron recombination/capture data
'H'	charge exchange recombination data from neutral hydrogen
'I'	electron impact ionisation data from stage below
'S'	electron impact ionisation data to stage above
'L'	unresolved dielectronic satellite line emission data

Table 2: Different types of transition in an ADF04 data set.

2.4 ADF07

Direct resolved electron impact ionisation coefficients

The data sets are collections of Maxwell averaged electron impact ionisation rate coefficients represented by the reactions

$$\begin{aligned} X_i^{z+} + \mathrm{e}^- &\rightarrow X_\rho^{(z+1)+} + \mathrm{e}^- + \mathrm{e}^-, \\ X_i^{z+} + \mathrm{e}^- \rightarrow X^{*(z)+} + \mathrm{e}^- &\rightarrow X_\rho^{(z+1)+} + \mathrm{e}^- + \mathrm{e}^-. \end{aligned} \tag{7}$$

That is the coefficients combine both direct ionisation and excitation/autoionisation. The tabulations are resolved by initial state i and final metastable ρ, with the initial state also mostly spanning just metastables. The rate coefficients are tabulated as a function of electron temperature. The data sets are typically grouped in sub-directories for a particular element. ADF07 is a fundamental data format. It should be noted that it does not include step-wise ionisation via multiple sequential excitations and then a final ionising collision. Effective ionisation coefficients, including step-wise ionisation, occur as a derived data output from collisional–radiative modelling and such data are archived as a sub-class of data format ADF11.

2.5 ADF08

Direct resolved radiative recombination coefficients

The data sets are collections of Maxwell-averaged radiative recombination coefficients (spontaneous free-bound transitions of Maxwellian electrons) represented by the reaction

$$X_\rho^{(z+1)+} + \mathrm{e}^- \rightarrow X_i^{z+} + h\nu. \tag{8}$$

The coefficients exclude recombination via resonance states, that is dielectronic recombination. The latter is normally presented as a separate process in the independent isolated resonance approximation (see ADF09). The coefficients are resolved by initial metastable ρ and final state i and are tabulated as a function of electron temperature. The data sets are normally grouped in sub-directories for different iso-electronic sequences (of the initial ion). Most describe recombination to a set of LS terms from the ground up to some limiting n-shell typically one or two above the ground and span just light elements. ADF08 is a fundamental data format. Effective recombination coefficients, including dielectronic recombination, three-body recombination, cascading and re-ionisation losses occur as a derived data output from collisional–radiative modelling and such data are archived as a sub-class of data format ADF11.

2.6 ADF09

Direct resolved dielectronic recombination coefficients

The data sets are collections of state-selective dielectronic recombination coefficients of Maxwellian free electrons. The process occurs via a radiative stabilisation of a doubly excited state formed by resonance capture, in competition with Auger breakup, and is represented by the reactions:

$$X_{\rho}^{(z+1)+} + \mathrm{e}^{-} \leftrightarrow X_{i,nl}^{z+} \rightarrow X_{\sigma,nl}^{z+} + h\nu \tag{9}$$

Non-resonant free electron capture (radiative recombination) is treated as a separate independent process (see ADF08). The coefficients are resolved by initial parent metastable ρ, final parent metastable core σ and captured electron $nl-$shell. Capture into low nl-shells is further resolved into terms or levels. The data sets are normally grouped in sub-directories for different iso-electronic sequences (of the initial ion). There are data sets both for term (LS) and intermediate (IC) coupling. Individual data sets are also separated by the type of parent transition ($\rho \rightarrow i$) according to the valence n-shell to which ρ and i belong. The data sets are tabulated as a function of electron temperature and the data are blocked for capture to resolved low levels (LS or IC), to high nl-shells (in the IC case) and to very high n-shells (LS and IC cases), depending on survival against secondary Auger breakup. The data sets span a wide range of elements up to zinc and span currently iso-electronic sequences up to Mg-like. These are complex data sets and the user is advised to read the detailed specification of ADF09 carefully. See also Badnell *et al* (2003) for more details on the treatment of dielectronic recombination within ADAS. ADF09 is a fundamental data format. Effective recombination coefficients, including dielectronic recombination, three-body recombination, cascading and re-ionisation losses occur as a derived data output from collisional–radiative modelling and such data are archived as a sub-class of data format ADF11.

2.7 ADF11

Iso-nuclear master files

The data sets provide a range of effective (collisional–radiative) coefficients which are required to establish the ionisation state of dominant ionic species and the radiative losses by these species, together with the energy balance of the free electrons, in a thermal plasma. Thus isonuclear master file data are split into a number of sub-classes as specified in table 3.

Mnemonic	Meaning
	Ionisation state determining coefficients driven by electrons interacting with dominant ions
ACD	Effective recombination coefficients
SCD	Effective ionisation coefficients
QCD	Cross-coupling coefficients
XCD	Parent cross-coupling coefficients
	Ionisation state determining coefficient driven by hydrogen interacting with dominant ions
CCD	Charge exchange effective recombination coefficients
	Radiated power and emission coefficients driven by electrons interacting with dominant ions
PLT	Line power driven by excitation of dominant ions
PRB	Continuum and line power driven by recombination and Bremsstrahlung of dominant ions
PLS	Line power from selected transitions of dominant ions
	Radiated power coefficient driven by hydrogen interacting with dominant ions
PRC	Line power due to charge transfer from thermal neutral hydrogen to dominant ions

Table 3: ADF11 format sub-classes

ADF11 is a derived data format. All the coefficients depend on free electron temperature and density and are calculated by collisional–radiative models. An ADF11 sub-class data set normally includes blocks for every ion of the element (excluding the neutral for recombination and the bare nucleus for ionisation). Data at two levels of refinement are present, namely, 'unresolved' (or 'stage-to-stage') in which only ground states of ions are assumed to be dominant species and 'metastable-resolved' in which both ground and metastable states of ions may be dominant. The former type are calculated with conventional collisional–radiative models and the latter by generalised-collisional–radiative (GCR) models. The data sub-classes QCD and XCD only apply in the GCR case. Also in the GCR case, the ion blocks in the sub-class data sets are subdivided for the different metastables. See Summers *et al* (2006) for the detailed theory and description of collisional–radiative modelling. Typical applications might be obtaining equilibrium ionisation balance fractional abundances, when only ACD and SCD are required, or solving 2-D impurity fluid dynamic transport models of tokamaks when ACD,

SCD and CCD are required as source terms in the number conservation equation and a linear combination of ACD, SCD, PLT, PRB (giving the electron energy loss) as a source term in the electron energy equation. The coefficients also apply to bifurcation choices in Monte Carlo modelling of impurity transport. Sub-directories of ADF11 are according to data sub-class and often by a two-digit year number. The year number represents year of introduction of an approximation. '89' is the wide coverage stage-to-stage data. '96' is the GCR data for light elements. See also section 2.1 for discussion on year numbers.

2.8 ADF12

Charge exchange effective emission coefficients

The data sets are collections of effective emission coefficients (given the mnemonic $\mathcal{QEF}$) for spectrum lines emitted by ions of elements following charge transfer from neutral beam donor atoms. For most data sets, the emitting ion is hydrogen-like (following capture by the bare nucleus) and each emissivity is the sum of the emissivities of all the component lines between two principal quantum shells at the centroid wavelength. ADF12 is a derived data format, in which a collisional–radiative model has been used to determine the populations of the emitting levels relative to the population of the recombining parent ion in its ground state (typically the bare nucleus) and the donor ion (typically a neutral beam atom). Thus the emissivity coefficient is defined with respect to unit neutral donor population and unit bare nucleus receiver population and is parametrically dependent on local beam energy, ion density, ion temperature and plasma Z_{eff} (and assumes plasma ion temperature is the same as electron temperature and electron density consistent with ion density and Z_{eff}). The span of spectrum lines in an AF12 data set always covers the visible spectral range, since the primary application of ADF12 is to visible charge exchange spectroscopy. There is an indexed data block for each spectrum line, with the coefficient data provided as separate one-dimensional scans in each parameter with respect to a reference value. Sub-directories of ADF12 are according to donor element and a two-digit year number. There are data for excited hydrogen donor states as well as ground and also for helium, lithium and sodium donors. The ADF12 data scope following closely that of the fundamental data format ADF01.

2.9 ADF13

Ionisation per photon coefficients

The data sets are collections of ionisation per photon quantities, given the mnemonic $\mathcal{S}/\mathcal{XB}$. Its reciprocal is called the 'photon efficiency'. An $\mathcal{S}/\mathcal{XB}$ is a quantity given for a specific spectrum line of an ion. It is useful in analysis of a spectrum line from an ionisation stage of an element, which is inflowing into a plasma from a surface, when the ionisation stage 'burns-through' fully to higher ionisation stages along the line of sight. Then the line-of-sight integrated intensity may be directly related to the influx of the element. The theory and application are described in Behringer *et al* (1989). ADF13 is a derived data format with $\mathcal{S}/\mathcal{XB}$ calculated from a collisional–radiative model. It is closely related to the SCD sub-class of format ADF11 and to the excitation $\mathcal{PEC}$s of format ADF15 described later — being essentially the ratio of the two. The collisional–radiative calculation is most appropriately carried out in the metastable-resolved GCR picture, with as many spectrum lines being needed to deduce the element influx as there are significant metastable populations in the analysed ion. The interpretation is a little subtle and it would be worthwhile to consult the reference above. There is an indexed block in the data set for each spectrum line (and for each metastable in the metastable-resolved case), with the tabulation an array in electron temperature and electron density. Sub-directories of ADF13 are according to iso-electronic sequence, with most available data being for light elements. The use of $\mathcal{S}/\mathcal{XB}$ has been particularly popular with visible wavelength lines, due to ease of observation and intensity calibration, but the data sets extend to short wavelength lines also.

2.10 ADF15

Photon emissivity coefficients

The data sets are collections of photon emissivity coefficients, given the mnemonic $\mathcal{PEC}$. Since the emission in a spectrum line $\epsilon_{i\to j}$ (photons cm^{-3} s^{-1}) is just the population number density ions (cm^{-3}) in the upper state of the transition times the spontaneous emission coefficient for the transition, the emissivity coefficients are obtained by relating the emission, via a collisional–radiative model, to the driving dominant populations. These may be the free electrons and the metastables of the ion itself via excitation, or the metastables of the parent ion, via free electron recombination. They may also be the thermal neutral hydrogen and the the metastables of the parent ion via charge exchange recombination. So the emission separates in general into three parts as

$$\epsilon_{i\to j} \;=\; \sum_{\sigma} \mathcal{PEC}^{(\mathrm{exc})}_{\sigma,i\to j} N_{\mathrm{e}} N^{z+}_{\sigma} + \sum_{\rho} \mathcal{PEC}^{(\mathrm{rec})}_{\rho,i\to j} N_{\mathrm{e}} N^{(z+1)+}_{\sigma}$$

$$+\sum_{\rho} \mathcal{PEC}^{(CX)}_{\rho,i\to j} N_{\rm H} N_{\sigma}^{(z+1)+} \tag{10}$$

and there are three types of $\mathcal{PEC}$ coefficients, and ADF15 is a derived data format with $\mathcal{PEC}$s calculated, most completely, from a generalised collisional–radiative model. An ADF04 data set is the input to the collisional–radiative calculation and so the scope of processes in that data set determines whether all of the three types of $\mathcal{PEC}$ are present in the resultant derived ADF15 data set or not. There is an indexed block in the data set for each spectrum line (and for each metastable in the metastable-resolved case and for each of the three types in general), with the tabulation an array in electron temperature and electron density. Sub-directories of ADF15 are according to iso-electronic sequence, with the most complete available data being for light elements. The ADF15 data sets really go along with the ADF11 data sets so that once the distribution of dominant ions in a plasma model is determined using ADF11 in a transport code, all the spectral emission may be predicted along lines-of-sight using ADF15. See Summers *et al* (2006) for more detail.

2.11 ADF21

Effective beam stopping coefficients

The data sets are collections of beam stopping coefficients, given the mnemonic $\mathcal{BMS}$. They are effective ionisation coefficients, including charge transfer losses, which leave the beam atoms ionised. The ionisation is due to collisions with ions in the plasma and free electrons, with the former more efficient at typical neutral heating beam energies. The ionisation losses are strongly influenced by the stepwise process and so the beam stopping coefficients are obtained from a collisional–radiative model. ADF21 is a derived data format. The stopping coefficients depend on the particular mixture of impurity ions present in the plasma. They are strongly parametrically dependent on the beam energy and the plasma ion densities and more weakly on plasma temperature. Data sets are for a single impurity (assumed fully ionised with their associated free electrons under charge conservation). A reference parameter set is specified and coefficient data are tabulated as an array in beam energy and density and as a vector in temperature, centred on the reference values. Stopping by a mixed impurity plasma is assembled as a linear combination of pure species stopping coefficients. It is recommended that the detailed prescription and use be examined with care. Conventionally beam stopping is related to the electron density, even though it is the ions which are the main influence, and that is what is done with ADF21.

See Anderson *et al* (2000) for more detail. ADF21 spans both hydrogen and helium with sub-directories for the different beam species and for different reference conditions (fast and and slow beams). The helium is treated as a metastable-resolved atom (ground and two metastables) and so it has further sub-directories for different GCR loss and cross-coupling coefficients.

2.12 ADF22

Effective beam emission/population coefficients

The data sets are collections of beam emission coefficients, given the mnemonic $\mathcal{BME}$. The processes and influences on the emission are the same as those responsible for beam stopping and the emission coefficients are obtained as a product of the same collisional–radiative models as the beam stopping coefficients. ADF22 is a derived data format and the data sets are structured in a similar manner to those of ADF21. Thus data sets are for a single impurity (assumed fully ionised with their associated free electrons under charge conservation) and for a specific spectrum line. A reference parameter set is specified and coefficient data are tabulated as an array in beam energy and density and as a vector in temperature, centred on the reference values. Emission by a mixed impurity plasma is assembled as a linear combination of pure species emission coefficients. It is recommended that the detailed prescription and use be examined with care. Beam emission is related to the electron density in ADF22 as for ADF21. ADF22 spans both hydrogen and helium with sub-directories for the different beam species and for different reference conditions (fast and and slow beams). For hydrogen beams, data are only given for H_α. For helium, there are additional sub-directories for a number of spectrum lines. The helium is treated as a metastable-resolved atom (ground and two metastables) as in ADF21 and so there are beam emission coefficient data sets relating to each of the metastables as a driver population. See Anderson *et al* (2000) for more detail on beam emission.

3 Indexing and the underlying database

OPEN-ADAS indexes the ADAS database for subsequent searching by scanning each ADAS data file (`.dat`) and extracting information about that file into a `.tag` file. These `.tag` files are then placed beside each `.dat` file on disk for inspection and cross-referencing purposes. A further process takes each `.tag` file and inserts the contents in a relational database structure suitable for web connectivity. Section 3.1 below describes the tagging procedure in detail and section 3.2 discusses the relational database.

3.1 Creation of tag files

The tagging system is implemented using the Perl programming language and works by recursively scanning through the ADAS directory tree working on each data class in turn. For each '`.dat`' file found, the program will generate a corresponding '`.tag`' file, this file is an XML representation indexing the data contained inside the data file[7]. A sample tag file for an ADF15 file is given in appendix A.

Perl was chosen for the indexing implementation because of its inbuilt support for string processing and manipulation, while each ADAS data file has a strict format for the main body of the file, the comments section is free-form[8] but contains information relevant to the indexing of the file and a language suited to the versatile treatment of strings has allowed for a much more rapid implementation than the use of a language such as Fortran. XML was chosen as the tagging format due to the wide-spread support for it within modern programming languages. We also note the recent data-centre development looking at the definition of an XML format for atomic data. OPEN-ADAS was not implemented with this in mind specifically but the choice of XML allows for an easier path to compare data, cross-reference and potential integration with other systems.

Each ADF has a bespoke Perl module written for it with two public subroutines, called, e.g. `adf15_process` and `adf15_insert`. The `adfNN_insert` routine will be discussed in section 3.2. The `_process` routine takes as a single argument the fully qualified name of an ADF file. The routine will then typically go through a number of steps:

1. parse the filename to extract any information,

2. parse the data in the file to extract information,

[7] The '`.tag`' file does not contain the data itself, merely information relevant to the indexing and searching of the data.

[8] Although a lot of the comments section are auto-generated.

3. check that the filename is consistent with the contents of the data,
4. parse the comments of the file to extract information,
5. check that the comments are consistent with the data,
6. check for the existence of '`.err`' file,
7. calculate an MD5SUM[9] for the file,
8. open up a file beside the '`.dat`' file with an extension of '`.tag`',
9. write the information to this file.

the implementation of each data file is, by the nature of the problem, quite unique but a number of common subroutines exist which many of the data class specific Perl modules utilise.

The indexing checks for 'contributors' to a specific ADF file, this is done in two main ways: (1) identification of initials in a filename or (2) the mention of a specific person's name in the comments section of the file. To facilitate this a lookup table of the various initials of contributors to the ADAS database is part of the indexing system. Also, patterns to match from the comments are also included in the indexing system, meaning that even if a name is written in different ways (e.g. 'A D Whiteford', 'Allan Whiteford', 'A Whiteford', etc.) they will appear consistently in the tag file, this allows for easier indexing within a relational database (see section 3.2). See appendix A for an example of the list of contributors to a file.

The indexing system also checks for 'predecessors', these are files in the ADAS database which the current file is derived from. For example, most ADF15 files originate from an ADF04 file also archived in central ADAS. Before the indexing system starts is collates a list of every file in the ADAS database, from that point on when scanning comment lines if it sees a file mentioned then it will list it as a predecessor. The indexing system also takes account of files having been created in a users own space and then archived within central ADAS (e.g. many of the GCR produced ADF15 files refer to ADF04 files in '`/home/mog`' which were subsequently archived within central ADAS, the indexing system can take account of this). See appendix A for an example of the list of predecessors for a file.

In addition to indexing all of the data, the tagging procedure also checks for consistency (as listed in the steps above). Where duplicate data exist in a file (e.g. the filename containing the element/charge as well as the content of

[9]This is a popular method of ensuring the integrity of files via a checksum, it also has inherent security features which are irrelevant to the current application.

the file) the tagging system will flag a warning and store this in an output file. The tagging system will also check for formatting errors. Many of the data corrections present in the release notes of ADAS v2.11 were due to errors flagged up by the tagging system.

By default the main indexing program will index each ADF class of relevance, however command line options exist to short-circuit this and only reprocess a particular ADF class or even a particular data file. This allows for rapid testing of the system when an error occurs and also for re-running checks on files which have been flagged as potentially inconsistent or as having a formatting error.

3.2 Relational database

As discussed above in section 3.1 each ADF-specific Perl module has a public `adfNN_insert` routine. This routine takes a '`.tag`' XML file and inserts it into a relational database implemented in MySQL[10]. The database schema is given in appendix B and is created separately to the insertion of data. The number of fields and records are given in table 4, it can be seen that the majority of the records are ADF09 states, these are the records of the initial and final states of the recombination processes which can be used for searching purposes.

There are two distinctions within the relational database, that of tables specific to a data class (denoted by a prefix of '`adfNN_`') and those which are general in nature, such as details about a file etc. Key tables are the 'ion' and 'filedetail' tables, the ion table contains information about which ion (i.e. element and charge) a particular ADF file is relevant to and 'filedetail' contains information on the location of the file, the filename, the type of file it is and its MD5SUM.

Two complications arise when moving the data from XML files into a relational database, namely the tracking of predecessors and the identification of contributors. Within the XML files these are stored as strings being either the full name of the person or the full path to a file. Within a RDBMS these should not be stored as filenames but rather pointers to other records, as an example if we take the example file of `adf15/pec96#c/pec96#c_pjr#c4.dat` and its predecessor, `adf04/adas#6/mom97_ls#c4.dat` then these have, respectively, internal IDs of 1921 and 3020. There then exists an entry in the 'predecessor' linking these two IDs: this is exemplified in table 5. In order for this to be possible the database must know the internal ID of each file as

[10]MySQL has been chosen due to the support and widespread use within the Linux community but it would be straightforward to switch over to a commercial database such as Oracle.

Table	Number of Fields	Number of Records
General		
beam	5	781
contributor	3	4,482
datatype	3	11
filedetail	8	4,380
ion	6	4,371
limits	25	4,378
people	3	27
predecessor	3	565
subtype	4	13
switches	6	2,720
Class Specific		
adf01_state	4	6,264
adf04_process	9	1,078
adf04_state	7	53,964
adf07_transition	10	711
adf08_state	10	2,233
adf08_transition	4	1,721
adf09_core	4	1,673
adf09_repn	3	74,589
adf09_state	8	952,299
adf12_transition	5	514
adf13_transition	15	7,829
adf15_transition	16	16,243
adf2122_transition	9	552
Total	170	1,141,398

Table 4: Summary of the number of fields (i.e. columns) and records (i.e. rows) in the OPEN-ADAS database. The tables listed at the top are specific to ADF classes while the table names listed at the bottom span multiple data classes.

it processes the XML '`.tag`' file. The database population hence happens in two steps, in the first step each '`.tag`' file is located an en entry made in the database simply giving the filename and path and at the same time generating an internal ID. On the second pass the data from the '`.tag`' files are inserted into the database and the predecessor table can also be populated since each internal ID is known. The only other way to achieve this would be to force the order of database population, this solution is impractical and inefficient.

Internal ID	Filename	Directory	Type
1921	`pec96#c_pjr#c4.dat`	`adf15/pec96#c`	15
3020	`mom97_ls#c4.dat`	`adf04/adas#6`	04

Internal ID	Parent File	Child File
232	3020	1921

Table 5: Example of predecessors being tied between different entries in the 'filedetail' table. The upper data show two entries from the 'filedetail' table with internal IDs of 1921 and 3020 and the second shows an entry from the 'predecessor' table which shows that `pec96#c_pjr#c4.dat` is descended from `mom97_ls#c4.dat`. Note that this allows for multiple descendants and ascendant per file.

The other complication, albeit simpler, is to match contributors to files. This is done by creating a list of possible contributors which is consistent with the list used in the tagging procedure (in fact they are different entry points to the same module). When this is done a mapping can be made from the internal ID of a file to the internal ID of a contributor.

We also note that there is a separate database within the implementation used for user accounts and for the web application to maintain a quasi-state, this is discussed in section 4.5 and appendix C.

4 Web interface

The user access to OPEN-ADAS is via a web based interface written in PHP. PHP was chosen due to the widespread support running on a Linux platform and it being one of the industry standard languages for web development. The output is standardised to W3C "XHTML 1.0 Transitional" and is formatted according to a CSS2 stylesheet. Adherence to web standards was judged to be of considerable importance to allow cross browser and cross platform accessibility. Table 6 shows some details of the browsers which were used in OPEN-ADAS testing.

Browser	Platform	Level of testing
Firefox 1	Linux	Extensive
Firefox 2	Linux	Extensive
Internet Explorer 6	Windows XP	Extensive
Internet Explorer 7	Windows XP	Moderate
Firefox 2	Windows XP	Moderate
Opera	Linux	Moderate
Safari	Mac OS X	Moderate
Firefox 3	Linux	Cursory
Opera-Mini	Smartphone	Cursory
Lynx	Linux	Cursory
Konqueror	Linux	Cursory

Table 6: Summary of browsers used in OPEN-ADAS testing along with platform details and the level (extensive, moderate or cursory) of testing which was performed.

The web interface allows the user to search for ADAS data in a number of different ways. Section 4.1 goes through each of the particular data classes in details giving information and examples on their custom search forms and also how the data are presented and available for downloading. Section 4.2 gives details on the display of predecessors, dependents and contributors. Section 4.3 gives details on how a user can search simultaneously across multiple data classes. Finally, section 4.4 discusses the 'freeform search' feature which provides a one field text interface to people which resembles a conventional internet search engine.

4.1 Specific ADAS data format descriptions

4.1.1 ADF01

Figure 2 shows the customised search for for ADF01 data (see also section 2.2). ADAS ADF01 files are targetted on fusion application so are organised in terms of a 'donor' beam ion and a 'target' plasma ion. Charge exchange cross-sections are, of course, only a function of two ions but ADAS does not seek to catalogue all cross-sections so does not need to organise its database in terms of 'ion 1' and 'ion 2'. Like all OPEN-ADAS forms, as much or as little information as desired can be entered by the user. For instance, if a target ion is not specified then all targets will be shown.

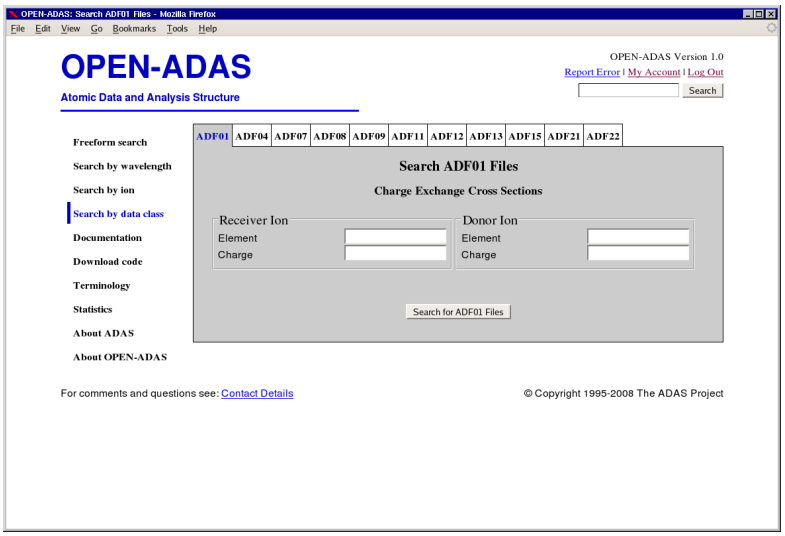

Figure 2: Screenshot of OPEN-ADAS showing the ADF01 searching form, the user can specify the receiver and donor of interest.

Figure 3 shows the results of searching for ADF01 files. In this case the search has been for a receiver ion of C^{6+} and a donor of any ions of hydrogen, this of course, only yields results for H^0. The search results page re-displays the form so that the user can make modifications if necessary. It then shows the list of ADAS files which were found matching the criteria. In this case 11 files were found. The receiver and donor for each file are printed along with the range of n which the file contains data for. Then a list of filenames are

displayed, clicking on these files will take the user to a page showing more details for that specific file.

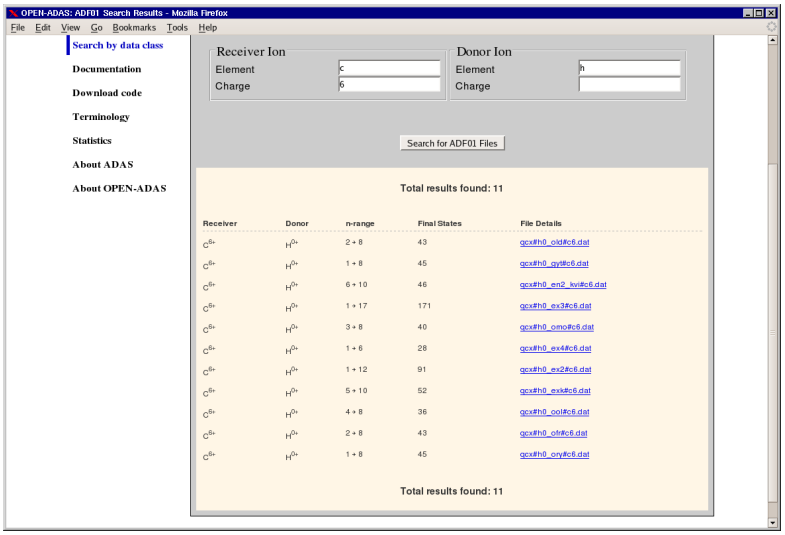

Figure 3: Screenshot of OPEN-ADAS showing ADF01 search results, here the search has been for a C^{6+} receiver and a hydrogen donor.

Figure 4 shows information on the file `qcx#h0_ory#c6.dat`. Some general information on the file is displayed on the top left of the information area, this specifies the receiver & donor ion, the energy range of the cross sections as well as the filename of the file and the full path within the ADAS database. To the right of this are options to download the ADAS data file, view the data inside the browser, download documentation on ADF01 files or software libraries (see section 5). Just below these are options to view comments or origins — see section 4.2 for more information on this feature.

Finally, a list of transitions are displayed. Note that in this case there exists a total cross section for the reaction as well as resolved cross sections to individual n levels of C^{5+} and to nl-resolved levels (e.g. C^{5+} (3p)).

4.1.2 ADF04

Figure 5 shows the customised search for for ADF04 data (see also section 2.3). ADF04 data are organised by particular ions and the form allows the

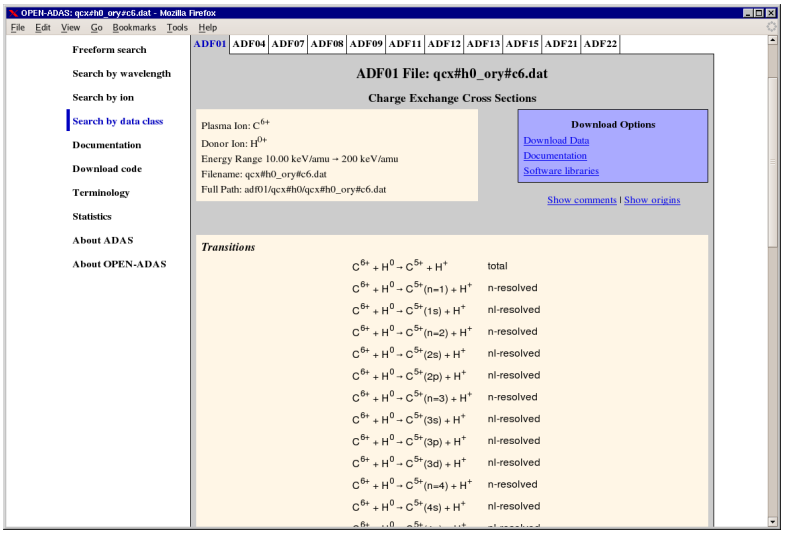

Figure 4: Screenshot of OPEN-ADAS showing the ADF01 file `qcx#h0_ory#c6.dat`, here the file contains both n- and nl-resolved cross sections.

user to specify the ion of interest. As with all OPEN-ADAS forms none of the fields are mandatory so if the user only puts in an element then all ionisation stages of the element will be search for. ADF04 files contain a number of processes (see section 2.3 and, in particular, table 2). Every ADF04 file contains free electron excitation but if a user wants to narrow their search to only files which contain certain processes then they can be selected here. If nothing is selected then all files will be searched. The options are inclusive in that ticking, e.g., charge exchange will return files which contain charge exchange data along with other processes.

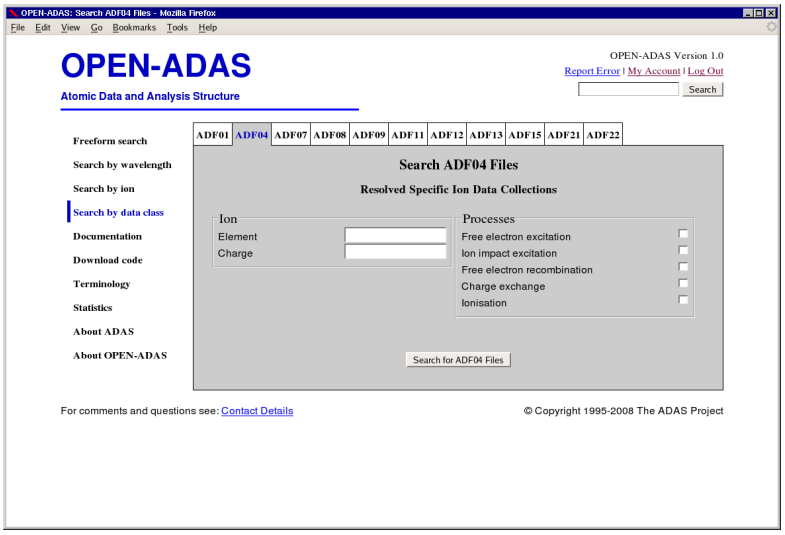

Figure 5: Screenshot of OPEN-ADAS showing the ADF04 searching form, the user can specify an ion of interest along with specific processes.

Figure 6 shows the results of searching for ADF04 files. The user has search for C^{3+} ADF04 files and has left the processes switches blank indicating they want to search for all data. As with all ADAS search pages, the form is redisplayed to the user so that they may make adjustments to it. Eleven ADF04 files have been found and they are listed below the original form. The ion for each match is shown along with the number of states in the file. Beside this is a table showing which processes are available in the ADF04 file. All ADF04 files contain electron impact excitation and it can be seen that some of the returned files contain recombination, some charge

exchange and some ionisation rates. None of the files returned here include ion impact excitation.

Finally, the filename itself is displayed, clicking on this filename will take the user to more details about a particular file.

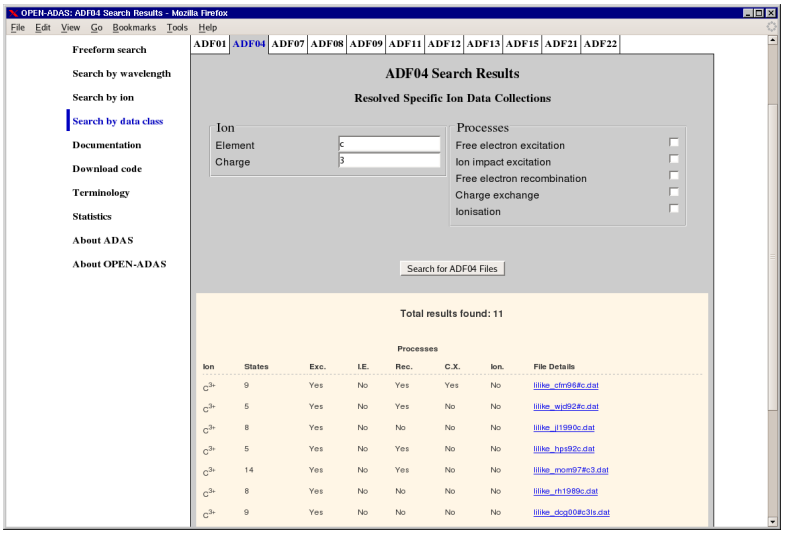

Figure 6: Screenshot of OPEN-ADAS showing ADF04 search results, here the search has been for C^{3+} data.

Figure 7 shows information on the file `lilike_cfm96#c.dat`. At the top left of the screen some general information is shown such as the ion contained in the file and the temperature range of the file as well as the filename of the file and the full path within the ADAS database. To the right of this are options to download the ADAS data file, view the data inside the browser, download documentation on ADF04 files or software libraries (see section 5). Just below these are options to view comments or origins — see section 4.2 for more information on this feature.

Below this information a list of the different types of transitions contained in the ADF04 file are given, the files themself typically contain numerous transitions for each type. Finally, a list of states are printed along with energy levels[11].

[11]It should be noted that energy levels in ADAS and OPEN-ADAS are not always spectroscopically accurate.

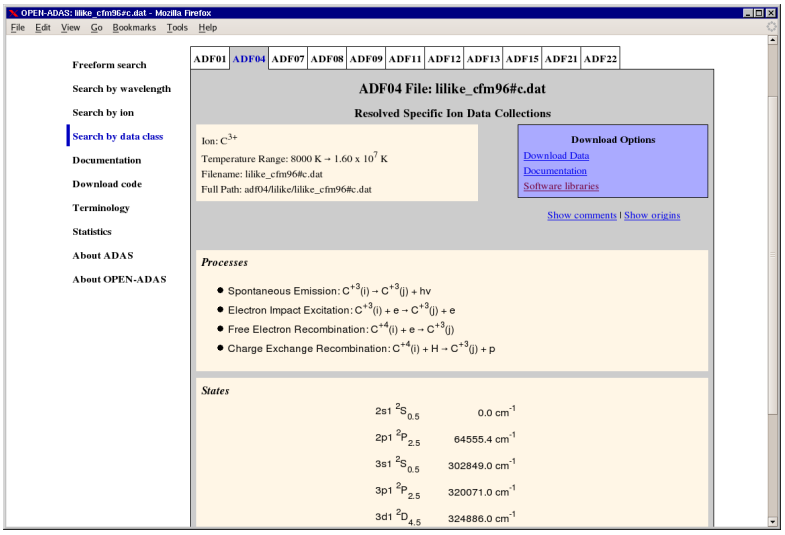

Figure 7: Screenshot of OPEN-ADAS showing the ADF04 file `lilike_cfm96#c.dat`. This file contains a number of processes which are shown along with energy level information.

4.1.3 ADF07

Figure 8 shows the customised search for for ADF07 data (see also section 2.4). The form is fairly simple in that only an element and charge are available for searching. Like all OPEN-ADAS forms, as much or as little information as desired can be entered by the user. For instance, if a particular charge is not specified then all ions of a particular element will be searched.

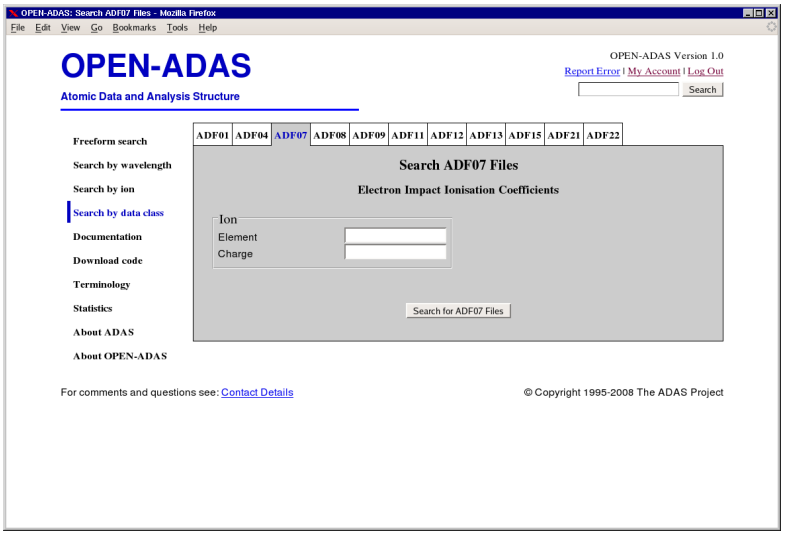

Figure 8: Screenshot of OPEN-ADAS showing the ADF07 searching form, the user can specify an element and charge state of interest.

Figure 9 shows the results of searching for ADF07 files. In this case the search has been for all ionisation stages of carbon. It can be seen that eight files have been found. Six of these files cover individual ions and the particular process is shown in the search results. The top two matches cover multiple ionisation stages in the same file which is indicated by specifying that the transition is for C^z. Beside each match are the number of transitions in the file, even for single ionisation stages there are multiple transitions as the data are metastable resolved. The filename of each file is also displayed, clicking on these files will take the user to a page showing more details for that specific file.

Figure 10 shows information on the file `szd93#c_c0.dat`. At the top left of the screen some general information is shown such as the ion contained in

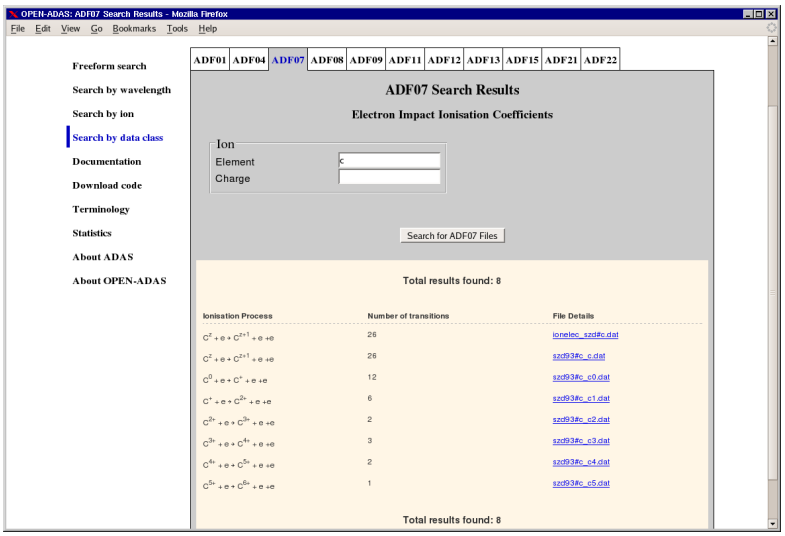

Figure 9: Screenshot of OPEN-ADAS showing ADF07 search results, here the search has been for all ionisation stages of carbon.

the file and the temperature range of the file as well as the filename of the file and the full path within the ADAS database. To the right of this are options to download the ADAS data file, view the data inside the browser, download documentation on ADF01 files or software libraries (see section 5). Just below these are options to view comments or origins — see section 4.2 for more information on this feature. Below this are the list of transitions in the file, this list specifies both initial and final state.

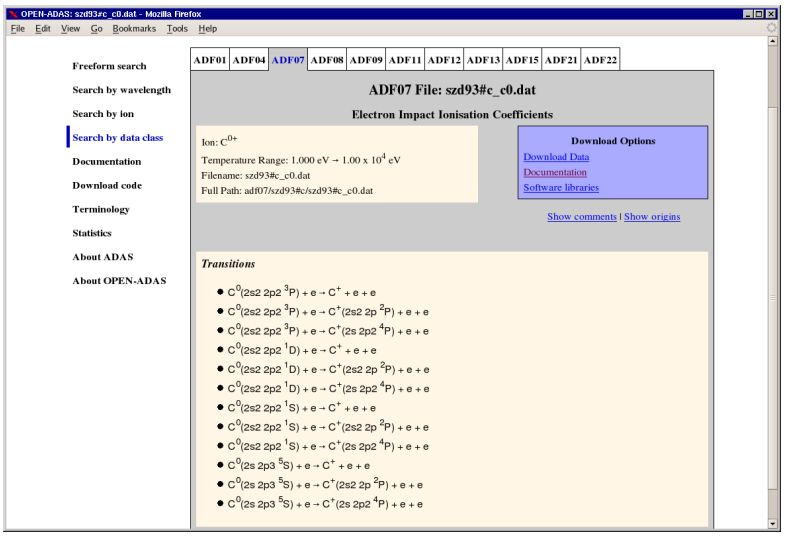

Figure 10: Screenshot of OPEN-ADAS showing the ADF07 file `szd93#c_c0.dat`, here the file contains twelve metastable-resolved transitions for C^0.

4.1.4 ADF08

Figure 11 shows the customised search for for ADF08 data (see also section 2.5). Like the ADF07 search facility, the form is fairly simple in that only an element and charge are available for searching. Like all OPEN-ADAS forms, as much or as little information as desired can be entered by the user. For instance, if a particular charge is not specified then all ions of a particular element will be searched.

Figure 12 shows the results of searching for ADF08 files. In this case the search has been for all ionisation stages of carbon. It can be seen that 18 files

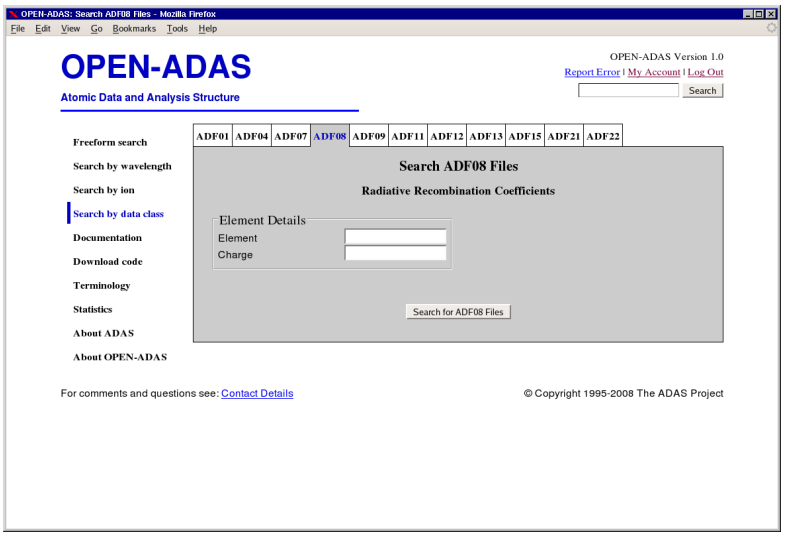

Figure 11: Screenshot of OPEN-ADAS showing the ADF08 searching form, the user can specify an element and charge state of interest.

have been found. For each file the particular transition is listed along with the number of parents (i.e. recombining) states and the number of target (i.e. recombined) states. The filename of each file is also displayed, clicking on these files will take the user to a page showing more details for that specific file.

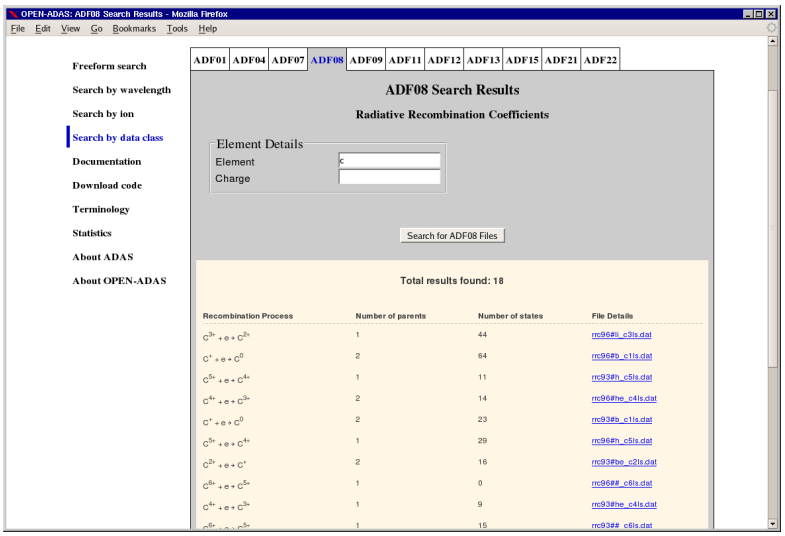

Figure 12: Screenshot of OPEN-ADAS showing ADF08 search results, here the search has been for all ionisation stages of carbon.

Figure 13 shows information on the file `rrc96#he_c4ls.dat`. At the top left of the screen some general information is shown such as the ion contained in the file and the temperature range of the file as well as the filename of the file and the full path within the ADAS database. To the right of this are options to download the ADAS data file, view the data inside the browser, download documentation on ADF08 files or software libraries (see section 5). Just below these are options to view comments or origins — see section 4.2 for more information on this feature. Below this are the list of the parent (i.e. recombining) states (typically metastables) and the recombined states. ADF08 data will contain transitions between these states.

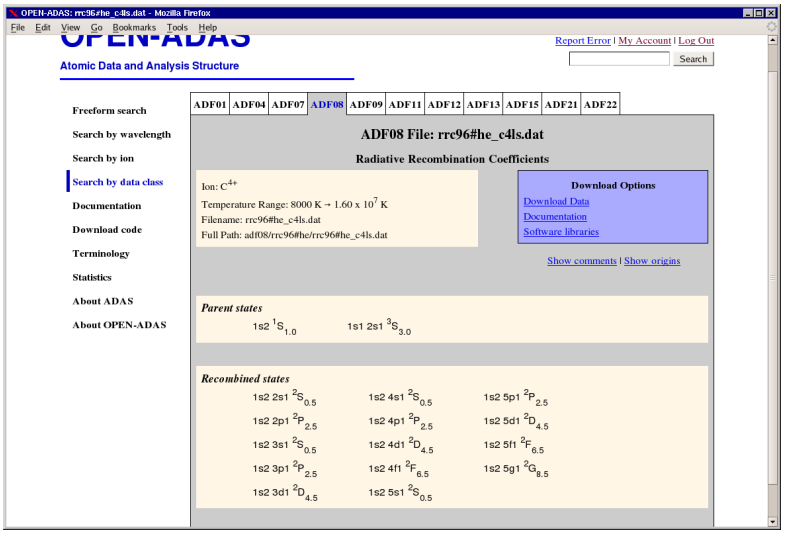

Figure 13: Screenshot of OPEN-ADAS showing the ADF08 file `rrc96#he_c4ls.dat`, here the file contains two parent states and fourteen recombined states for C^4.

4.1.5 ADF09

Figure 14 shows the customised search for for ADF09 data (see also section 2.6). The form allows the user to specify an element and charge along with a year number (see section 2.1 for more information on ADAS terminology relating to year numbers) for the data. It's also possible to specify if LS or IC coupling is required and also the core transition for the ADF09 files; ADAS DR data are split by core excitation — see section 2.6 for more details. Like all OPEN-ADAS forms, as much or as little information as desired can be entered by the user.

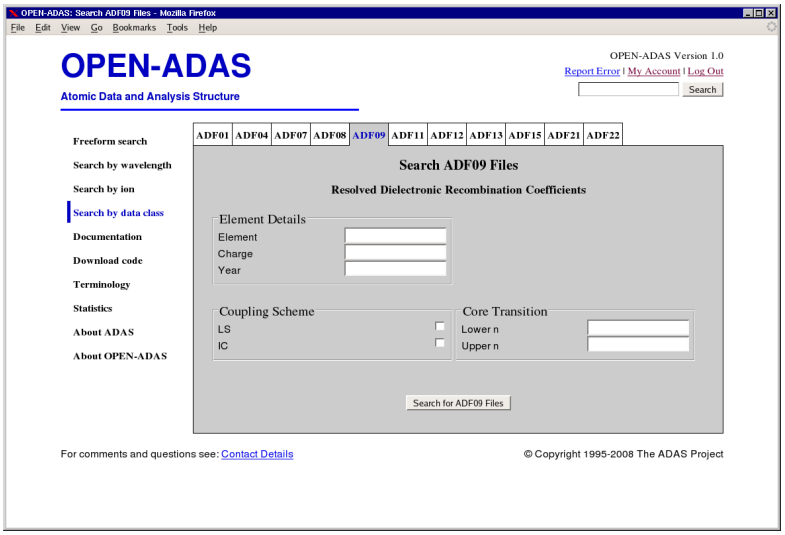

Figure 14: Screenshot of OPEN-ADAS showing the ADF09 searching form, the user can specify an ion of interest along with a year designation, a coupling scheme and core excitation.

Figure 15 shows the results of searching for ADF09 files. In this case the search has been for all ionisation stages of carbon but for only IC coupled data. It can be seen that 16 files have been found. For each file the ion is listed along with the year, coupling scheme and the core excitation (see section 2.6 for more details on these). The filename of each file is also displayed, clicking on these files will take the user to a page showing more details for that specific file.

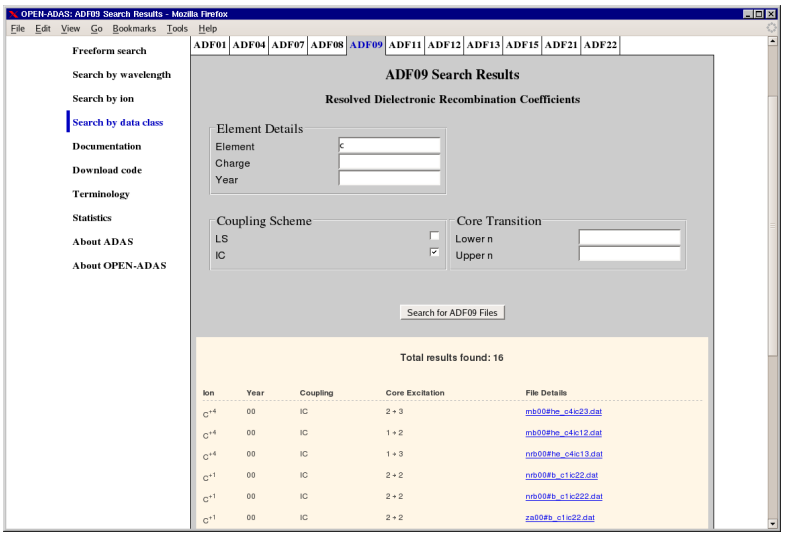

Figure 15: Screenshot of OPEN-ADAS showing ADF09 search results, here the search has been for IC coupled data for all ionisation stages of carbon.

Figure 16 shows information on the file `mb00#he_c4ic12.dat`. At the top left of the screen some general information is shown such as the ion contained in the file and the temperature range of the file as well as the filename of the file and the full path within the ADAS database. To the right of this are options to download the ADAS data file, view the data inside the browser, download documentation on ADF09 files or software libraries (see section 5). Just below these are options to view comments or origins — see section 4.2 for more information on this feature.

Below this information is a list of representative n-shells which build upon the parent states. There are also a specific list of low-level recombined states. See section 2.6 for a fuller description of what ADF09 files contain.

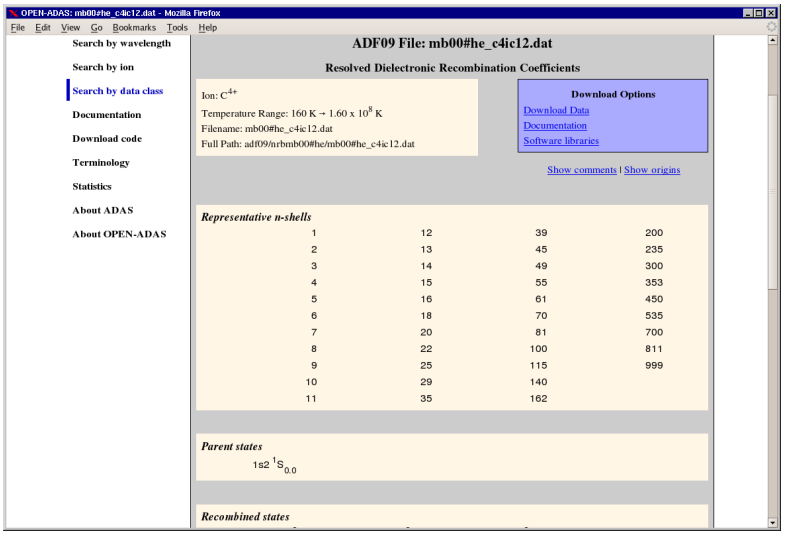

Figure 16: Screenshot of OPEN-ADAS showing the ADF09 file `mb00#he_c4ic12.dat`, here the file contains one parent state and many recombined states.

4.1.6 ADF11

Figure 17 shows the customised search for for ADF11 data (see also section 2.7). The form allows the user to specify the element of interest as well as the year marker and metastable resolution (see section 2.1 for details on the

meaning of metastable resolution and year markers). Below these options are boxes for the user to specify which subtype of ADF11 file they are interested in — see section 2.7 for a discussion of the different types of data.

Like all OPEN-ADAS forms, as much or as little information as desired can be entered by the user. For instance, if a particular charge is not specified then all ions of a particular element will be searched. Similarly, if no specific types of data are searched for then all types will be returned.

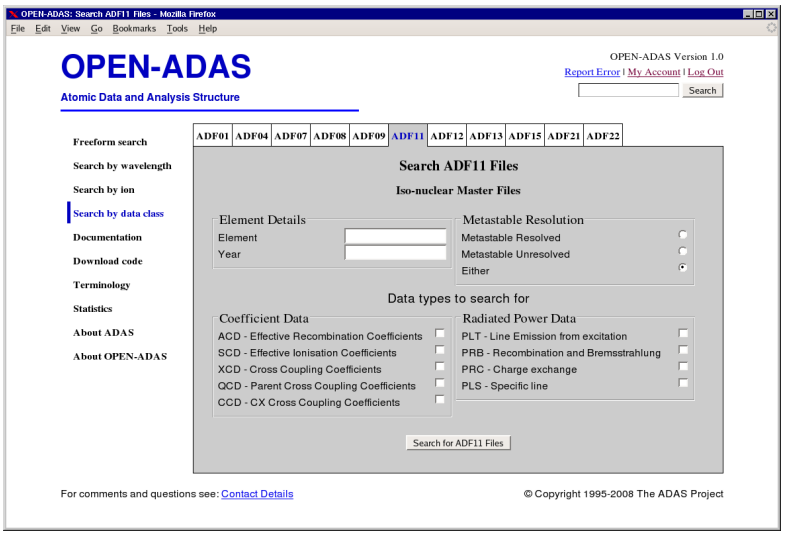

Figure 17: Screenshot of OPEN-ADAS showing the ADF11 searching form, see text for details.

Figure 18 shows the results of searching for ADF11 files. In this case the search has been for ACD, SCD, XCD and QCD files for carbon. It can be seen that for the Unresolved case only ACD and SCD files exist but for the resolved case there are matches for ACD, SCD, XCD and QCD. For each file found the specifics of the file are printed along with the filename. Clicking on the filename will take the user to a page showing more details for that specific file.

Figure 19 shows information on the file `acd96r_c.dat`.

At the top left of the screen some general information is shown such as the ion contained in the file and the temperature & density range of the file as well as the filename of the file and the full path within the ADAS database.

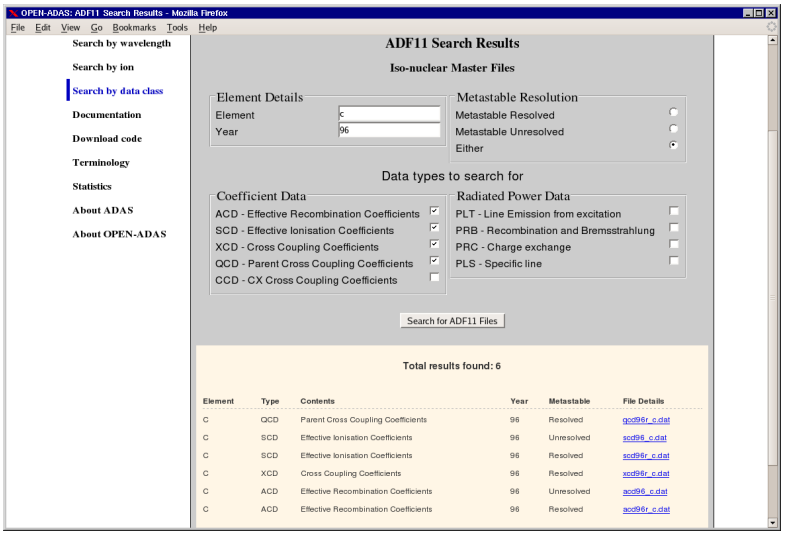

Figure 18: Screenshot of OPEN-ADAS showing ADF11 search results, here the search has been for carbon data.

To the right of this are options to download the ADAS data file, view the data inside the browser, download documentation on ADF11 files or software libraries (see section 5). Just below these are options to view comments or origins — see section 4.2 for more information on this feature. In this case the options to via origins and comments have been enabled and additional information is displayed.

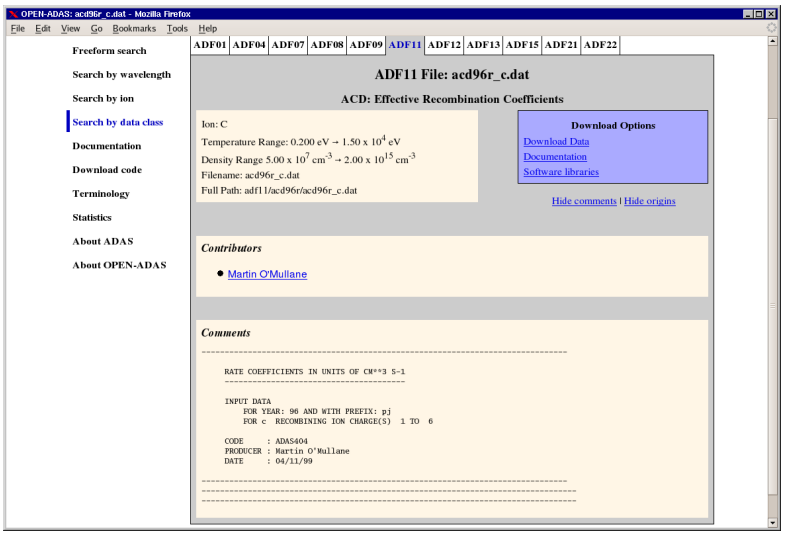

Figure 19: Screenshot of OPEN-ADAS showing the ADF11 file `acd96r_c.dat`, also shown are the comments and contributors — see section 4.2 for more information on contributors.

4.1.7 ADF12

Figure 20 shows the customised search for for ADF12 data (see also section 2.8). The form allows the user to specify the element and charge of interest. Since ADF12 data are related to emission the user can also specify a minimum and maximum wavelength for this emission.

Below these options is the option to resolve results by 'transition' or 'file'. If the user picks 'transition' then every matching transition is displayed, typically ADF12 files contain multiple transitions so this means that files will often appear more than once. If the user selects 'file' then each file will

only appear once, in this case the wavelength search criteria is still used but matches over the whole file.

Like all OPEN-ADAS forms, as much or as little information as desired can be entered by the user. For instance, if no wavelength range is specified then all transitions from a particular element or ion will be displayed.

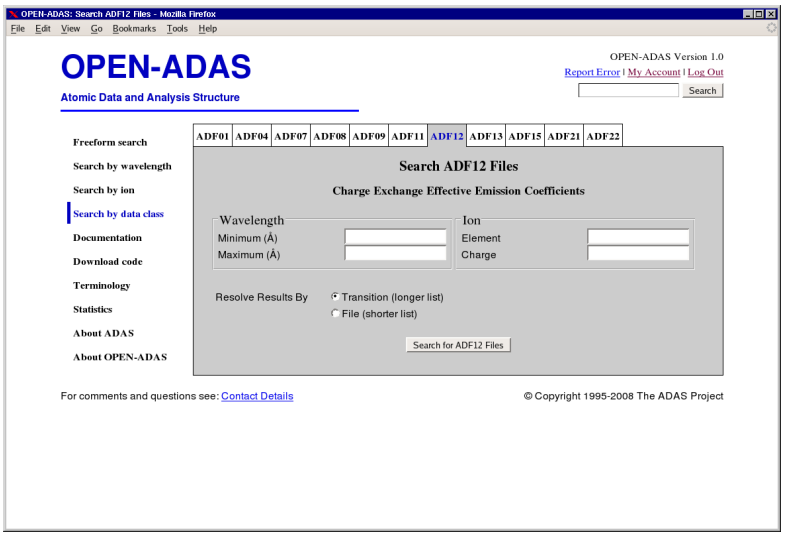

Figure 20: Screenshot of OPEN-ADAS showing the ADF12 searching form, see text for details.

Figure 21 shows the results of searching for ADF12 files. In this case the user has searched for carbon data between 4000Å and 6000Å. The user has opted to see results by transition. Note than two main transitions are found, the $10 \rightarrow 8$ transition at 4498.9Å and the more familiar $8 \rightarrow 7$ transition at 5290.7Å. Both of these results occur in multiple files so each file is listed separately. Note also that the ADF12 files typically contain both transitions so each file is also listed twice. Clicking on the filename will take the user to a page showing more details for that specific file. Note that if the user had opted to search by 'file' rather than wavelength the the layout of the results is different since individual transitions are no longer identified.

Figure 22 shows information on the file `qef93#h_c6.dat`. At the top left of the screen some general information is shown such as the ion contained in the file and the parameter ranges covered by the file — temperature, density,

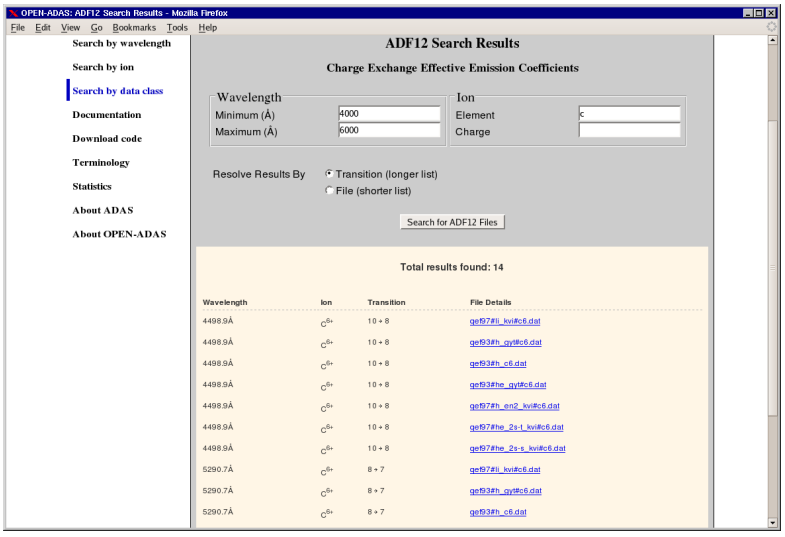

Figure 21: Screenshot of OPEN-ADAS showing ADF12 search results, here the search has been for carbon data between 4000Å and 6000Å.

beam energy, magnetic field strength and Z_{eff}. Also in this are the filename of the file and the full path within the ADAS database. To the right of this are options to download the ADAS data file, view the data inside the browser, download documentation on ADF12 files or software libraries (see section 5). Just below these are options to view comments or origins — see section 4.2 for more information on this feature. Below the general information is a list of transitions contained in the file along with their wavelengths.

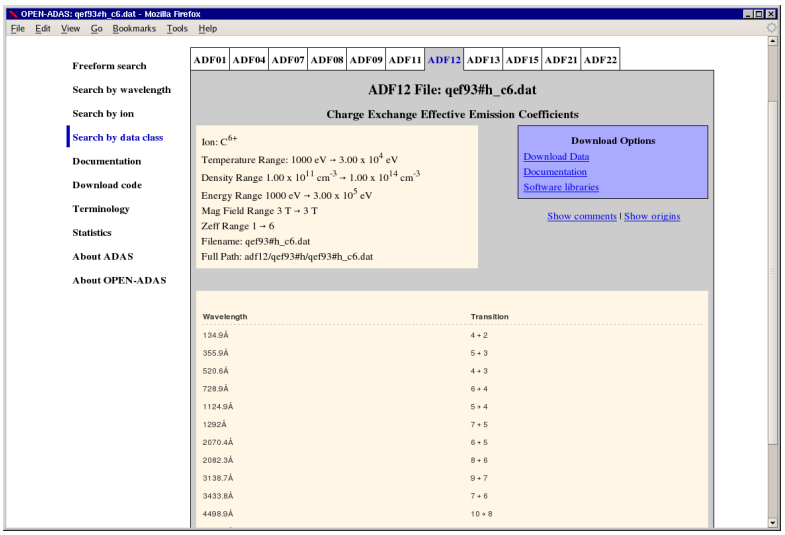

Figure 22: Screenshot of OPEN-ADAS showing the ADF12 file `qef93#h_c6.dat` along with the transitions present in the file.

4.1.8 ADF13

Figure 23 shows the customised search for for ADF13 data (see also section 2.9) which is identical to the ADF12 form. The form allows the user to specify the element and charge of interest. Since ADF13 data are related to emission the user can also specify a minimum and maximum wavelength for this emission.

Below these options is the option to resolve results by 'transition' or 'file'. If the user picks 'transition' then every matching transition is displayed, typically ADF13 files contain multiple transitions so this means that files

will often appear more than once. If the user selects 'file' then each file will only appear once, in this case the wavelength search criteria is still used but matches over the whole file.

Like all OPEN-ADAS forms, as much or as little information as desired can be entered by the user. For instance, if no wavelength range is specified then all transitions from a particular element or ion will be displayed.

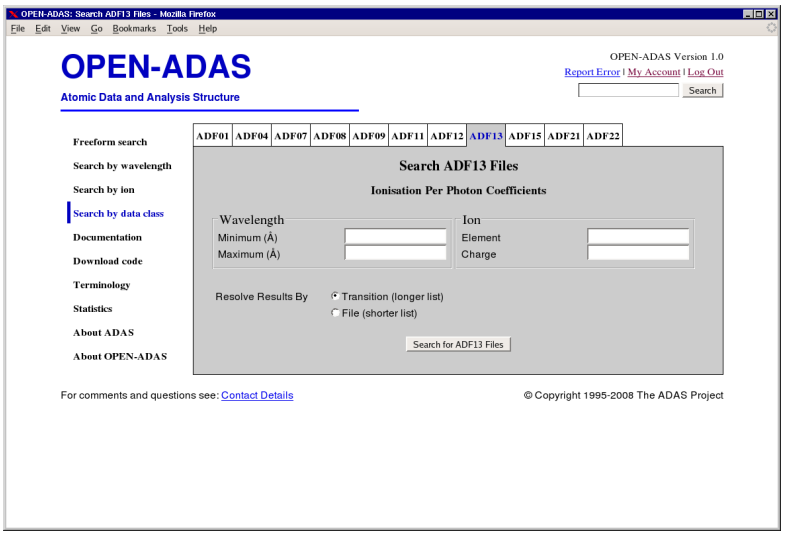

Figure 23: Screenshot of OPEN-ADAS showing the ADF13 searching form, see text for details.

Figure 24 shows the results of searching for ADF13 files. In this case the user has searched for neutral carbon data between 4000Å and 6000Å. The user has opted to see results by transition. Multiple transitions are shown and it can be seen that only two distinct files are shown on the results page, had the user opted to see results by 'file' then only two results would have been shown but no transition information would have been present. Clicking on the filename will take the user to a page showing more details for that specific file. Note that if the user had opted to search by 'file' rather than wavelength the the layout of the results is different since individual transitions are no longer identified.

Figure 25 shows information on the file `sxb96#c_vsr#c0.dat`. At the top left of the screen some general information is shown such as the ion

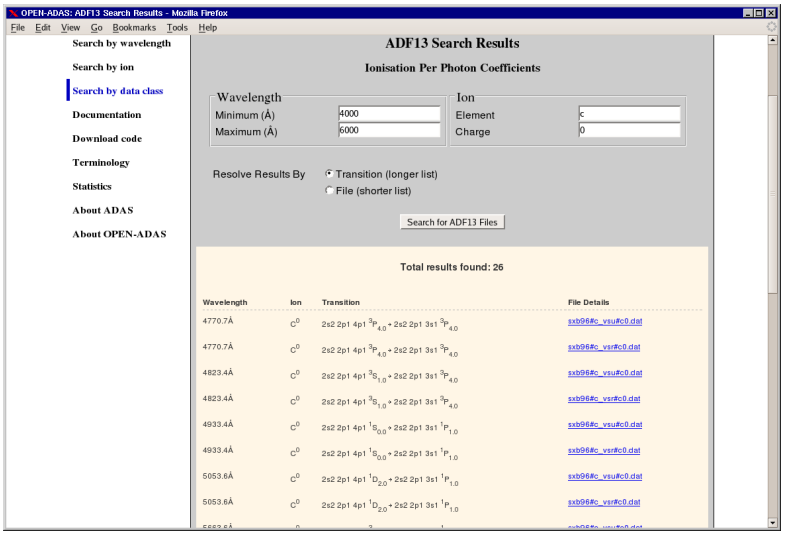

Figure 24: Screenshot of OPEN-ADAS showing ADF13 search results, here the search has been for neutral carbon data between 4000Å and 6000Å.

contained in the file and the temperature & density range of the file as well as the filename of the file and the full path within the ADAS database. To the right of this are options to download the ADAS data file, view the data inside the browser, download documentation on ADF13 files or software libraries (see section 5). Just below these are options to view comments or origins — see section 4.2 for more information on this feature. In this case the options to via origins and comments have been enabled and additional information is displayed.

Finally each transition in the file is listed. Note that the file being shown is metastable resolved so for each transition there are four entries, one for each of the C^{0+} driving populations — see section 2.1 for more information about metastable resolution in ADAS.

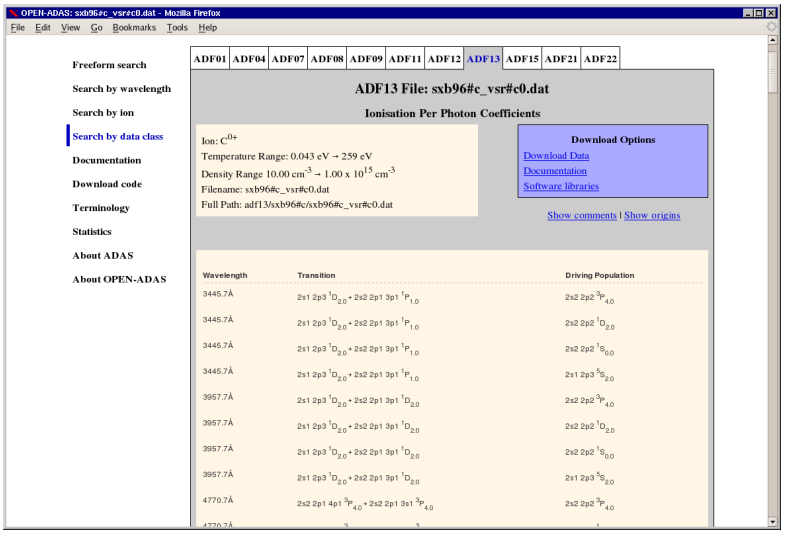

Figure 25: Screenshot of OPEN-ADAS showing the ADF13 file `sxb96#c_vsr#c0.dat` along with the transitions present in the file.

4.1.9 ADF15

Figure 26 shows the customised search for for ADF15 data (see also section 2.10) which is identical to the ADF12 and ADF13 forms. The form allows the user to specify the element and charge of interest. Since ADF15 data

are related to emission the user can also specify a minimum and maximum wavelength for this emission.

Below these options is the option to resolve results by 'transition' or 'file'. If the user picks 'transition' then every matching transition is displayed, typically ADF15 files contain multiple transitions so this means that files will often appear more than once. If the user selects 'file' then each file will only appear once, in this case the wavelength search criteria is still used but matches over the whole file.

Like all OPEN-ADAS forms, as much or as little information as desired can be entered by the user. For instance, if no wavelength range is specified then all transitions from a particular element or ion will be displayed.

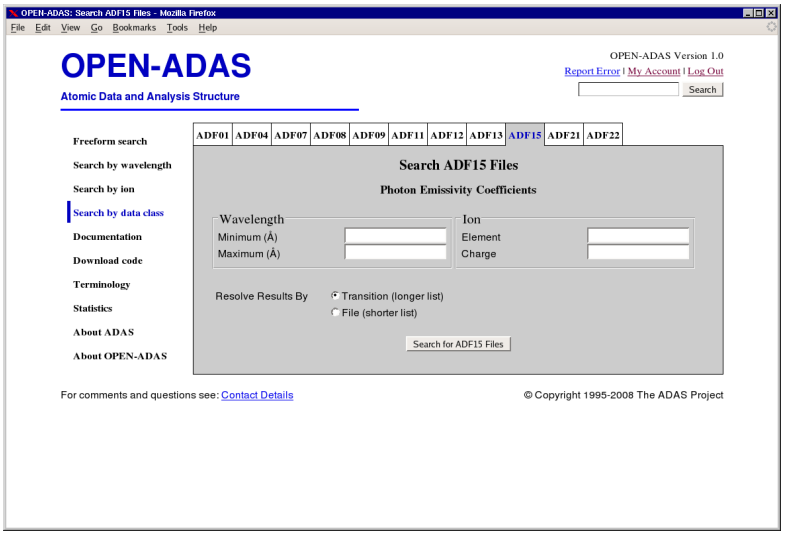

Figure 26: Screenshot of OPEN-ADAS showing the ADF15 searching form, note that

Figure 27 shows the results of searching for ADF15 files. In this case the user has searched for carbon data between 4000Å and 5000Å. The user has opted to see results by transition. Multiple transitions are shown and it can be seen that only two distinct files are shown on the results page, had the user opted to see results by 'file' then only two results would have been shown but no transition information would have been present. Clicking on the filename will take the user to a page showing more details for that specific

file. Note that if the user had opted to search by 'file' rather than wavelength the the layout of the results is different since individual transitions are no longer identified.

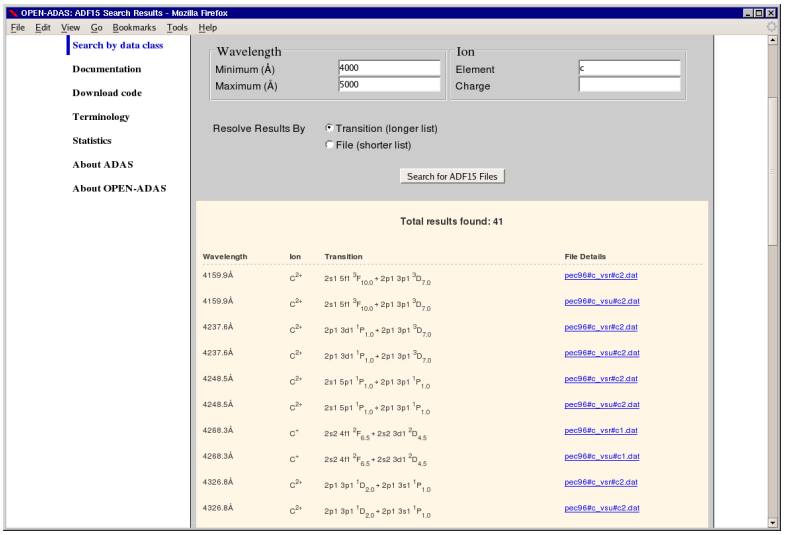

Figure 27: Screenshot of OPEN-ADAS showing ADF15 search results, here the search has been for carbon transitions between 4000Å and 5000Å.

Figure 25 shows information on the file `pec96#c_vsr#c2.dat`. At the top left of the screen some general information is shown such as the ion contained in the file and the temperature & density range of the file as well as the filename of the file and the full path within the ADAS database. To the right of this are options to download the ADAS data file, view the data inside the browser, download documentation on ADF15 files or software libraries (see section 5). Just below these are options to view comments or origins — see section 4.2 for more information on this feature. In this case the options to via origins and comments have been enabled and additional information is displayed.

Finally each transition in the file is listed. Note that the file being shown is metastable resolved so for each transition there are four entries, two for each of the driving populations from excitation of C^{2} (see section 2.1 for more information about metastable resolution in ADAS), one for emission due to charge exchange and one for emission due to recombination. See section 2.10

for a discussion of the different types of emission in an ADF15 file.

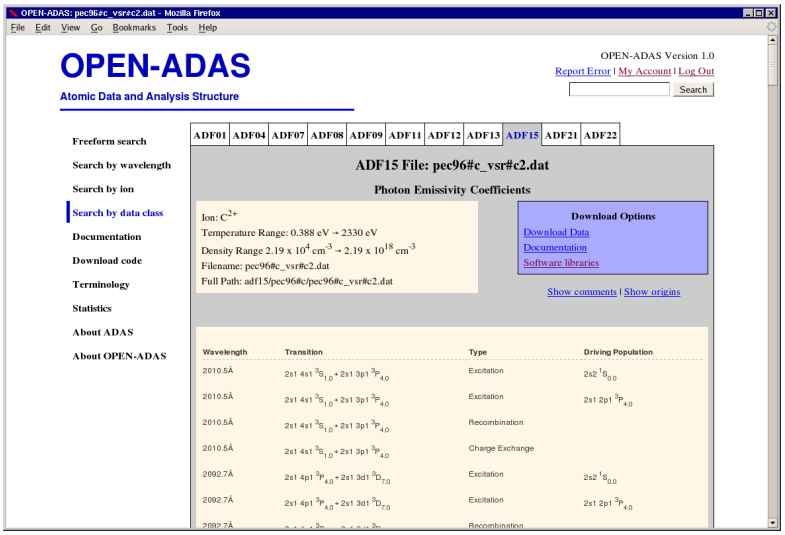

Figure 28: Screenshot of OPEN-ADAS showing the ADF15 file `pec96#c_vsr#c2.dat` along with the transitions present in the file.

4.1.10 ADF21

Figure 29 shows the customised search for for ADF21 data (see also section 2.11). ADAS ADF21 files are targetted on fusion application so are organised in terms of a 'donor' beam ion and a 'target' plasma ion. The user can also specify if they are interested in only beam stopping coefficients or only cross-coupling coefficients (see section 2.11 for a discussion of these). Like all OPEN-ADAS forms, as much or as little information as desired can be entered by the user. For instance, if a target ion is not specified then all targets will be shown. In addition, if the user does not supply a preference regarding the type of data then both datatypes will be searched.

Figure 30 shows the results of searching for ADF21 files. In this case the search has been for a receiver ion of C^{6+} and a donor of hydrogen. Information is displayed on the plasma and beam species as well as the contents of the file. A list of filenames are displayed, clicking on these files will take the user to a page showing more details for that specific file.

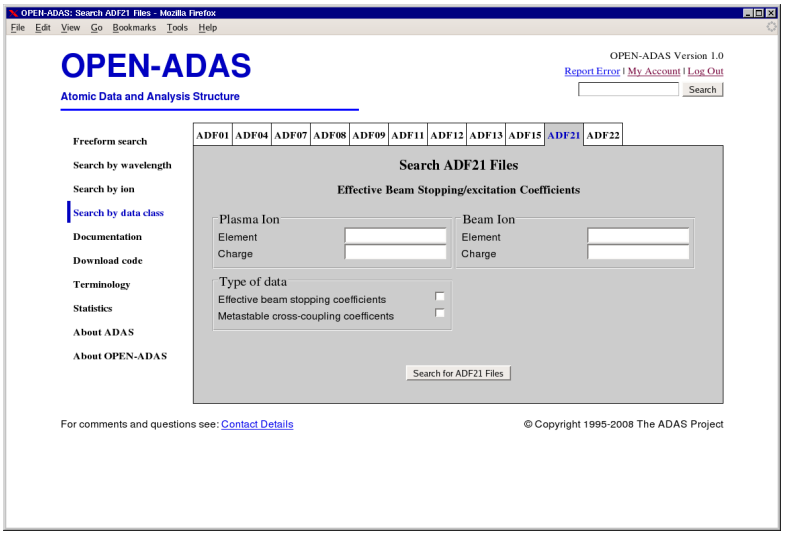

Figure 29: Screenshot of OPEN-ADAS showing the ADF21 searching form, note that

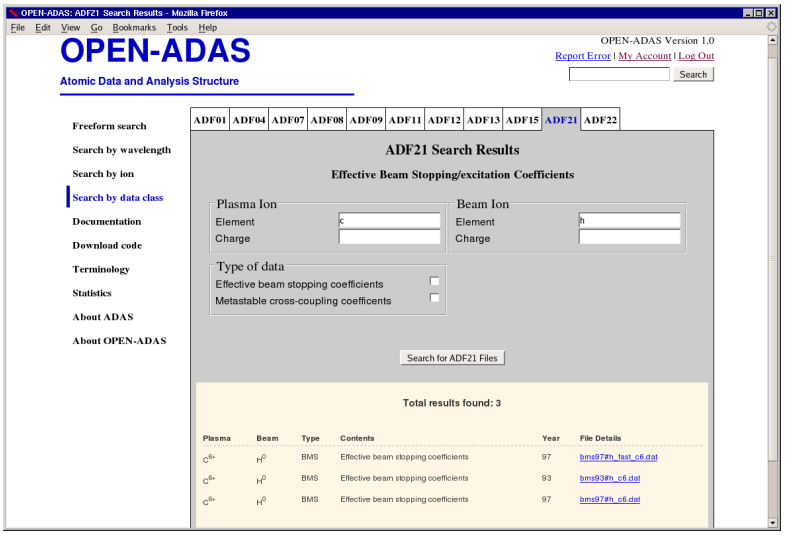

Figure 30: Screenshot of OPEN-ADAS showing ADF21 search results, here the search has been for

Figure 31 shows information on the file `bms97#h_c6.dat`. Some general information on the file is displayed on the top left of the information area, this specifies the receiver & donor ion, the temperature, density & energy range of the cross sections as well as the filename of the file and the full path within the ADAS database. To the right of this are options to download the ADAS data file, view the data inside the browser, download documentation on ADF21 files or software libraries (see section 5). Just below these are options to view comments or origins — see section 4.2 for more information on this feature.

ADF21 files are a combination of 1D and 2D scans from a set of reference parameters, these reference parameters are also displayed. Finally the nominal processes are shown, the contents of ADF21 files are fully density dependent collisional–radiative quantities so the processes shown are indicative of what the file specifies rather than the fundamental processes actually stored in the file.

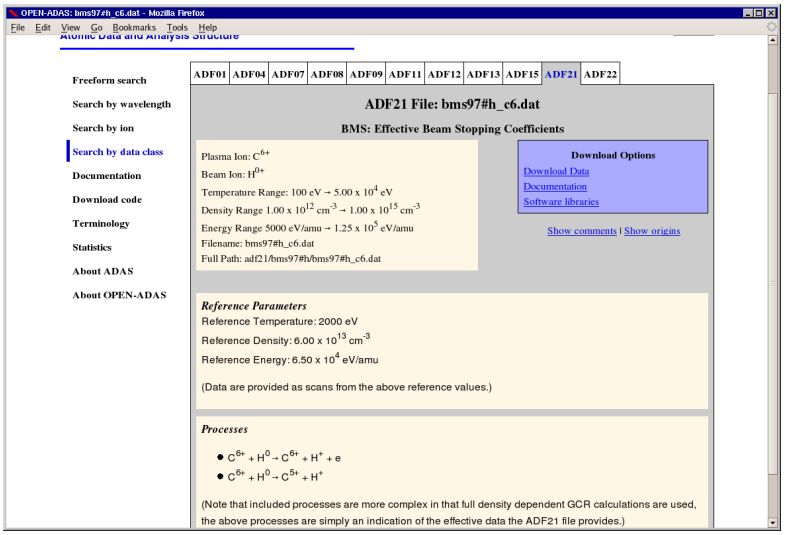

Figure 31: Screenshot of OPEN-ADAS showing an ADF21 file, here the file contains

4.1.11 ADF22

Figure 32 shows the customised search for for ADF22 data (see also section 2.12). ADAS ADF22 files are targetted on fusion application so are organised in terms of a 'donor' beam ion and a 'target' plasma ion. The user can also specify if they are interested in only beam emission coefficients or only beam populations (see section 2.12 for a discussion of these). For the case of beam emission it's also possible for the user to specify a wavelength range. Like all OPEN-ADAS forms, as much or as little information as desired can be entered by the user. For instance, if a target ion is not specified then all targets will be shown. In addition, if the user does not supply a preference regarding the type of data then both datatypes will be searched.

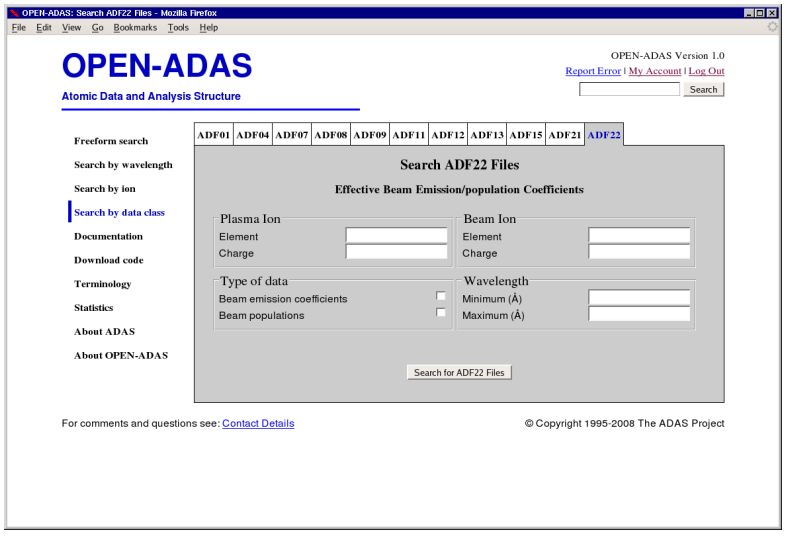

Figure 32: Screenshot of OPEN-ADAS showing the ADF22 searching form, note that

Figure 33 shows the results of searching for ADF21 files. In this case the search has been for a receiver ion of C^{6+} and a donor of hydrogen. Information is displayed on the plasma and beam species as well as the contents of the file — it can be seen that both emission and populations have been found. A list of filenames are displayed, clicking on these files will take the user to a page showing more details for that specific file.

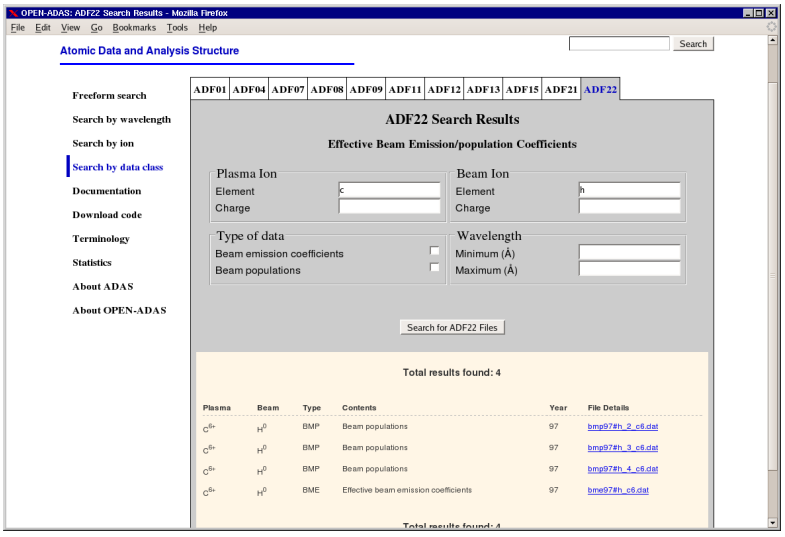

Figure 33: Screenshot of OPEN-ADAS showing ADF22 search results, here the search has been for

Figure 34 shows information on the file `bme97#h_c6.dat`. Some general information on the file is displayed on the top left of the information area, this specifies the receiver & donor ion, the temperature, density & energy range of the cross sections as well as the filename of the file and the full path within the ADAS database. To the right of this are options to download the ADAS data file, view the data inside the browser, download documentation on ADF22 files or software libraries (see section 5). Just below these are options to view comments or origins — see section 4.2 for more information on this feature.

ADF22 files are a combination of 1D and 2D scans from a set of reference parameters, these reference parameters are also displayed. Finally the nominal processes are shown, the contents of ADF22 files are fully density dependent collisional–radiative quantities so the processes shown are indicative of what the file specifies rather than the fundamental processes actually stored in the file.

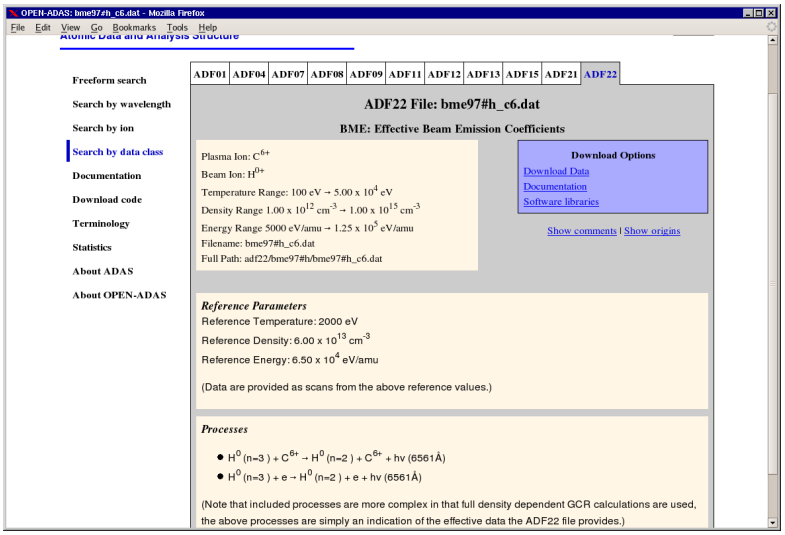

Figure 34: Screenshot of OPEN-ADAS showing an ADF22 file, here the file contains

4.2 Predecessors and dependents

Figure 35 shows viewing the ADF04 file `mom97_ls#c4.dat` with the option to view origins turned on - this is activated by the link which normally says 'Show Origins' but which turns to 'Hide Origins' when selected.

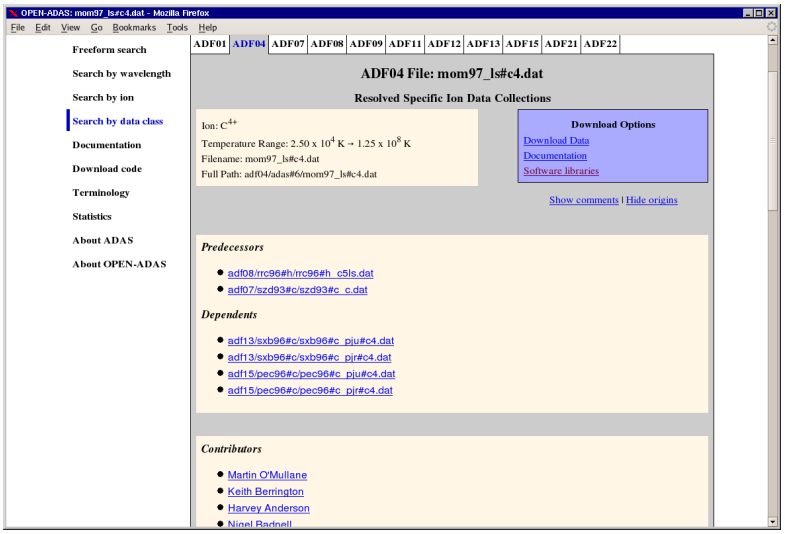

Figure 35: Screenshot of OPEN-ADAS showing the ADF04 file `mom97_ls#c4.dat` to illustrate the role of predecessors and dependents in OPEN-ADAS.

It can be seen that the files which `mom97_ls#c4.dat` depend on are shown, these are the ADF08 and ADF07 files `rrc96#h_c5ls.dat` and `szd93#c_c.dat` respectively. The system also shows the files in the ADAS database which are built upon this ADF04 file, these are two ADF13 files and two ADF15 files. All of these files can be selected and the user is directed to the relevant page to show information on them. See section 3.1 for more details on how the predecessors and dependents are identified and stored.

Below the predecessors and dependents a list of 'contributors' are displayed (again see section 3.1 for more details on how contributors are identified). These are people who have contributed to the data in the file `mom97_ls#c4.dat`. These names can also be selected and the user will be taken to a page showing all of the files that person has contributed to. For

example, figure 36 shows all of the files which have been contributed to by Costanza Maggi.

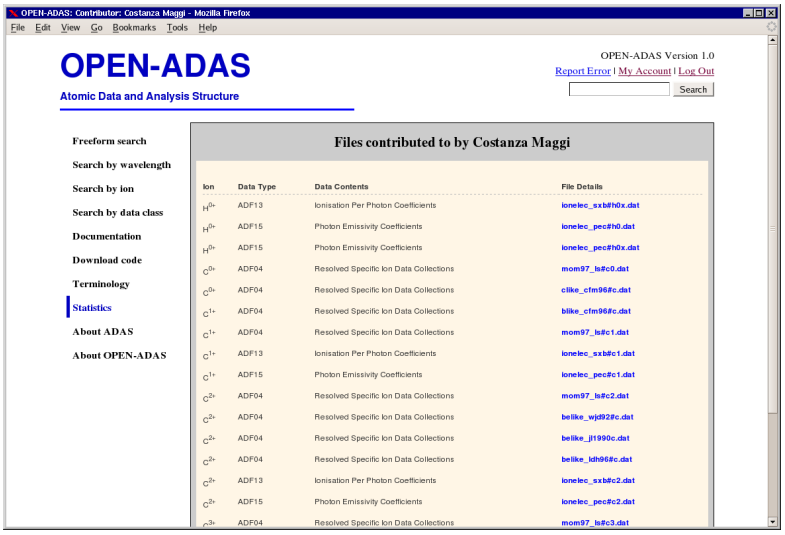

Figure 36: Screenshot of OPEN-ADAS showing the list of files which Costanza Maggi has contributed to.

Please note that the predecessor and contributors system is not definitive and the canonical information on the sources of data in a file are contained in the comments. The comments are plain text and appear at the bottom of every ADAS file and can also be viewed online by selecting the 'View Comments' option.

4.3 Cross-dataclass searching

As well as the specific dataclass searches as given in section 4.1 it's also possible to search OPEN-ADAS across a number of data classes simultaneously. These are detailed below.

4.3.1 Search by ion

Figure 37 shows the form for searching OPEN-ADAS by ion. It's possible for the user to specify a list or range of elements. Both boxes are optional. Table 7 gives some examples of searches which can be performed.

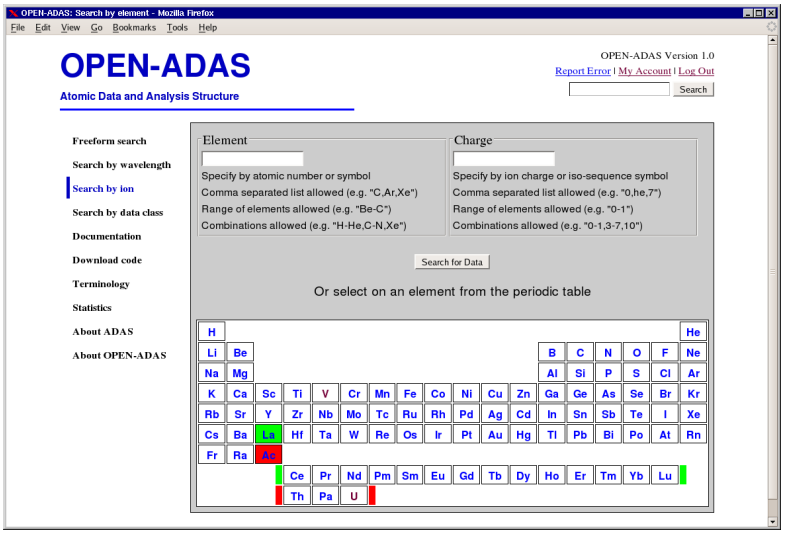

Figure 37: Screenshot of OPEN-ADAS showing the search by ion feature.

Element	Charge	Searches for
C	3	All C^{3+} data
	0	Neutral data for all elements
C		All carbon data
C	0-3	Neutral data to three times ionised data for carbon
C-Ar	he	All helium-like data for carbon to argon
C-O,Kr	he-be	He-like to be-like data for C, N, O and Kr

Table 7: Examples of searching by ion, the 'element' and 'charge' columns correspond to the fields in the OPEN-ADAS search form. Note that in some of the examples the fields are left blank

The search by ion feature allows a user to get an overview of the contents of OPEN-ADAS. The feature is also useful if the user is unsure of the different types of ADAS data class and which one is best. Figure 38 shows an example of such a search

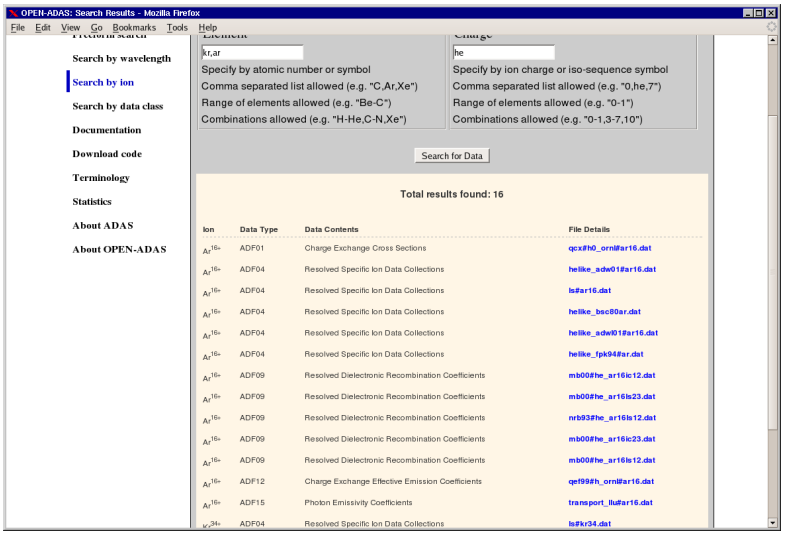

Figure 38: Screenshot of OPEN-ADAS showing the search by ion feature, here the user has searched for helium-like krypton and argon. Results from different ADAS data classes are displayed.

4.3.2 Search by wavelength

For a user who is interested in a specific spectral region or who is unaware of the various ADAS data formats and their complexities it is possible to simply search by a wavelength range. Figure 39 shows such a search. This search mechanism searches for transitions in ADF12 (charge exchange emission), ADF13 (S/XB emission), ADF15 (photon emissivity coefficients) and ADF22 (beam emission) files and displays them on one page.

The feature allows a user to get a broad idea of the types of emission in a particular range but we do note that ADAS and OPEN-ADAS often doesn't contain spectroscopically accurate wavelengths and we would recommend NIST for line identification, this feature of OPEN-ADAS is simply to

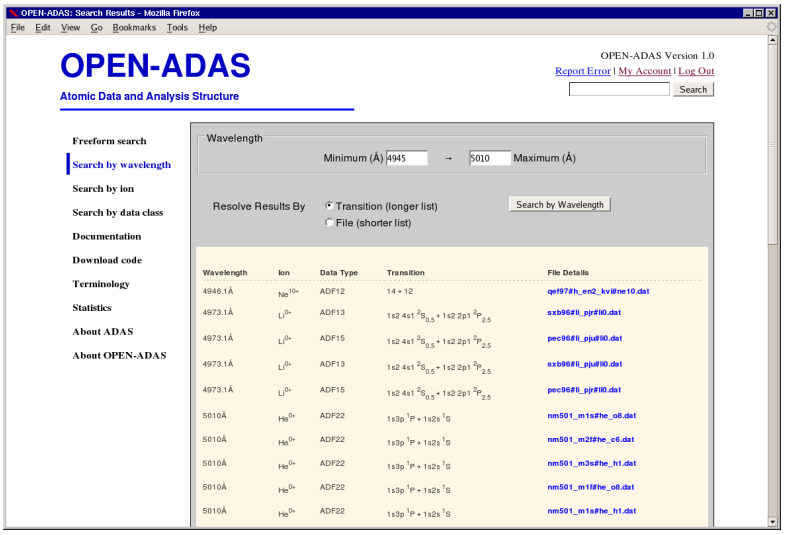

Figure 39: Screenshot of OPEN-ADAS showing the search by wavelength feature. The user has selected a wavelength range of 4945Å to 5010Å and multiple results have been displayed.

facilitate a rapid overview of available data.

4.4 Freeform search

OPEN-ADAS allows a freeform search feature. This presents a single text box to the user allowing for a single text entry. This is more in keeping with a conventional modern search engine interface (e.g. Google, Yahoo!, MSN search). The text string is parsed to extract out ions of interest, wavelength ranges etc. As well as element names and symbols a number of key words are recognised by the system, these are given in table 8.

Figure 40 shows an example of the freeform search system being used. The user has asked to know about neutral Be influx in the visible part of the spectrum. OPEN-ADAS has returned S/XB coefficients for Be^{0+} and highlighted the visible transitions.

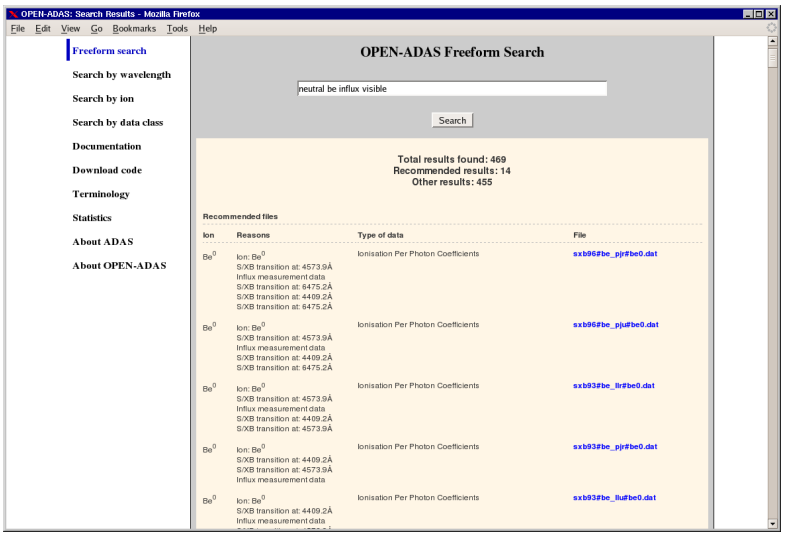

Figure 40: Screenshot of OPEN-ADAS showing the freeform search feature, here the user has typed in 'neutral be influx visible' and relevant results have been shown.

Table 9 gives some short examples of the freeform searching facility. These examples are simply illustrative of the applicability of the freeform searching mechanism. The system has been designed to be as flexible as possible.

Word	Meaning
beam	Preceding specification was for beam species
visible	Wavelength range of 4000Å–6500Å
x-ray	Wavelength range of 0.1Å–100Å
sxr	Wavelength range of 1Å–100Å
soft x-ray	Wavelength range of 1Å–100Å
ir	Wavelength range of 6500Å–9500Å
infra-red	Wavelength range of 6500Å–9500Å
infra red	Wavelength range of 6500Å–9500Å
uv	Wavelength range of 1000Å–4000Å
ultra-violet	Wavelength range of 1000Å–4000Å
ultra violet	Wavelength range of 1000Å–4000Å
euv	Wavelength range of 1000Å–4000Å
vuv	Wavelength range of 1000Å–4000Å
emission	ADF12, ADF13 and ADF15
beam emission	BME data in ADF22
influx	ADF13
recombination	ADF08 and ADF09
dr	ADF09
dielectronic recombination	ADF09
rr	ADF08
radiative recombination	ADF08
cx	ADF01, ADF12 and CCD/PRC in ADF11
charge exchange	ADF01, ADF12 and CCD/PRC in ADF11
charge transfer	ADF01, ADF12 and CCD/PRC in ADF11
ionisation	ADF07 data
ionization	ADF07 data
eii	ADF07 data
attenuation	BMS data in ADF21
stopping	BMS data in ADF21
population	ADF04
pop	ADF04
power	PLT, PLS, PRB and PRC in ADF11
radiation	PLT, PLS, PRB and PRC in ADF11
radiated	PLT, PLS, PRB and PRC in ADF11

Table 8: Summary of specific words, acronyms etc. which OPEN-ADAS understands and their meaning to the system.

Search	Meaning
"whiteford"	All files contributed to by Allan Whiteford
"Fe23"	All Fe^{23+} data
"FeXXIV"	All Fe^{23+} data
"1-4A"	Emission between 1Å and 4Å
"1-4nm"	Emission between 1nm and 4nm
"Fe24 1-4A"	Fe^{24+} emission between 1Å and 4Å
"he beam c"	Data on a helium beam interacting with a carbon impurity
"he beam emission carbon 5000A-7000A"	Data on emission from a helium beam between 5000Å and 7000Å driven by a carbon impurity in a plasma
"oxygen 4000A"	Emission from oxygen around 4000Å
"xe dr"	Dielectronic recombination data for xenon

Table 9: Examples of freeform searches and their meanings in the OPEN-ADAS system. As can be seen the searches can be quite complex. This list is not exhaustive and combinations and extensions of the above searches will also work.

The freeform search system contains the concept of best matches and partial matches. If a user searches for, e.g. , "xe dr" than all the xenon files are found along with all the DR files. Where these two sets overlap we say they are the recommended results. After these results partial results will be listed. In this case the partial results will be all the xenon files in the database (with the exception of files already displayed) followed by all the DR files in the database.

If the system is not able to match every word then the subset with the highest number of matches are the recommended results. For example, in the search "be influx 50A" it is not possible to return an exact match. The recommended match would then be (1) all of the Be S/XB data, (2) any S/XB data around 50Å and (3) any Be emission around 50Å. In this case there is no match for (3) so the results would display all of the Be S/XB data followed by some neon S/XB data (which emits at around 50Å). The ordering of the recommended and partial matches are based on the ordering of the original users search terms.

4.5 User management and options

Users of OPEN-ADAS must login to download data, they need to create an account as shown in figure 41. The information collected in this process is

not sent to third parties but it's stated that aggregate data (e.g. total number of users) may be made public during the signup process.

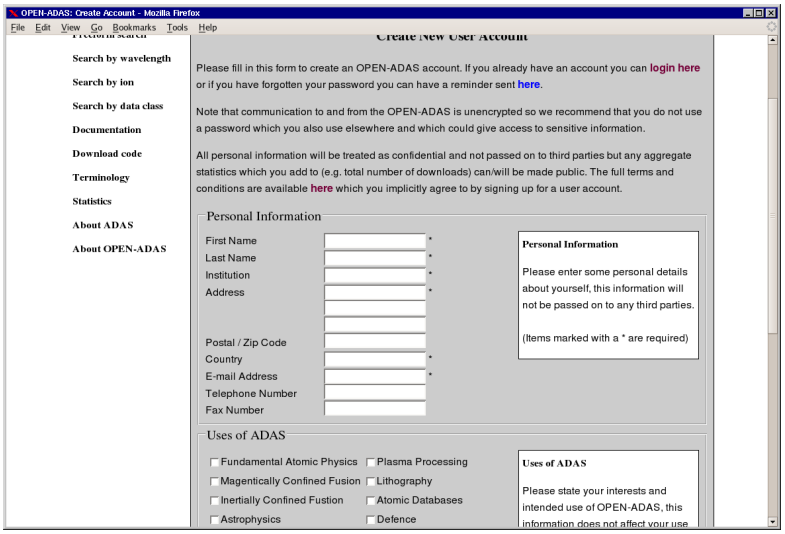

Figure 41: Screenshot of OPEN-ADAS showing the account creation page, more information such as a desired username and password are supplied further down the form.

Anytime a user tries to access a page which requires a login, the screen shown in figure 42 is shown. After the user has entered their details they will be sent back on to the page they were looking for.

When a user is logged in, they can access the "My Account" section from a link at the top right of the page. This allows them to manage their details, review their activity on the OPEN-ADAS site and also set various preferences. The preferences page is shown in figure 43.

The user account details are held in a separate database, the schema for this database is given in appendix C.

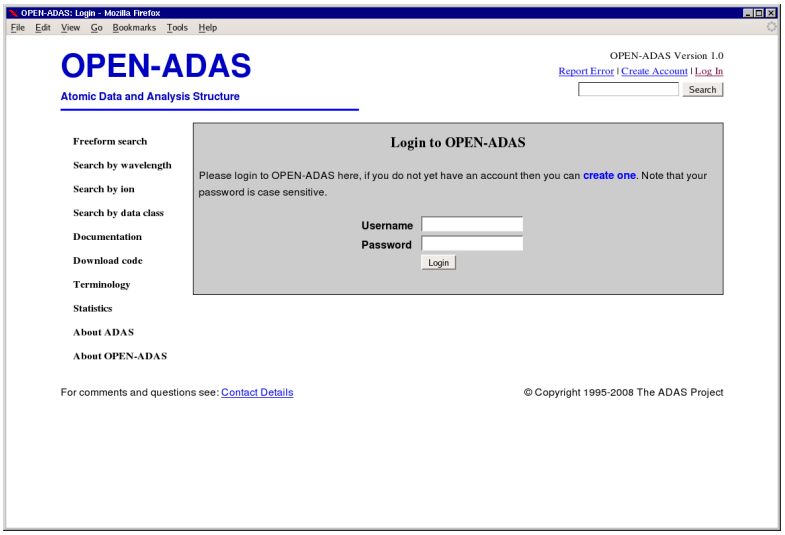

Figure 42: Screenshot of OPEN-ADAS showing the login screen, a link to the create account screen is also available.

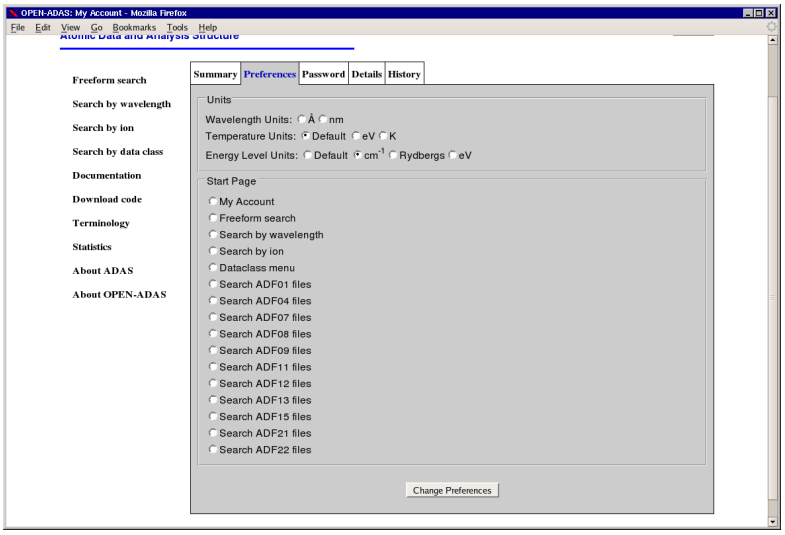

Figure 43: Screenshot of OPEN-ADAS showing the user preferences section, units of wavelength, temperature and energy can be chosen as well as the default start page.

5 Software libraries and documentation

For each of the eleven data classes released with OPEN-ADAS there are associated software routines and documentation released. The documentation files correspond to sub-appendices from the ADAS manual and are specific to each data class. These give in detail the precise formatting of each file and the general status of the data. They are available from the "Documentation" section of the site.

The downloadable code are from the central ADAS Fortran libraries. Routines to read ADAS data are named `xxdata_NN.for` where `NN` is the format of the file. Source code is given for each of the core reading routines as well as supplementary Fortran routines which are necessary for operation. The files are distributed as gzipped tar files and are designed to run on a UNIX platform. Table 10 gives a list of the files contained in the `xxdata_04.tar.gz` file.

File	Contents/Purpose
`README`	File explaining contents of each file
`LICENSE`	License information (see also appendix G)
`COMPILING`	Information on compiling the subroutine
`xxdata_04.pdf`	Documentation for the subroutine
`xxdata_04.for`	Main user-level subroutine
`i4fctn.for`	Subroutine necessary for operation of `xxdata_04`
`i4idfl.for`	Subroutine necessary for operation of `xxdata_04`
`i4unit.for`	Subroutine necessary for operation of `xxdata_04`
`r8fctn.for`	Subroutine necessary for operation of `xxdata_04`
`xxcase.for`	Subroutine necessary for operation of `xxdata_04`
`xxpars.for`	Subroutine necessary for operation of `xxdata_04`
`xxprs1.for`	Subroutine necessary for operation of `xxdata_04`
`xxrmve.for`	Subroutine necessary for operation of `xxdata_04`
`xxslen.for`	Subroutine necessary for operation of `xxdata_04`
`xxword.for`	Subroutine necessary for operation of `xxdata_04`
`test.for`	Small example test program (see appendix H)
`test.sh`	Test script to compile and run `test.for`
`test.dat`	Test ADF04 file for `test.for` to read

Table 10: Contents of `xxdata_04.tar.gz`, each file is listed along with the contents and purpose of the file.

6 Conclusions

OPEN-ADAS makes available a substantial body of fundamental and derived atomic data. These data are selected and designed for application to the modelling and analysis of ionisation state and spectral emission from plasmas. Relevant plasmas span wide ranges of temperature and density and the OPEN-ADAS derived data are distinctive in their attention to the dependence on density.

OPEN-ADAS database is built from collections of data, organised in ADAS data formats. These collections are internally complete, in terms of criteria specified in the data sets. For application, the completeness is often more important that the fact that any one piece of data, such as a single transition collisional rate coefficient, is of the highest available precision. ADAS data formats frequently have sub-directories or year numbers assigned to particular methodologies (and consequently average precision level).

Data sets all have 'comment' sections at the end. It is important that the OPEN-ADAS user takes note of these comments which include attributability, antecedents, date of production and further guidance information.

A number of routines and procedures are provided for reading ADAS data formats. These are freely available for download and their use is recommended. The specifications of some ADAS data formats have extended over the years; not all data sets exploit the full specifications which can be elaborate. The supplied routines and procedures handle the full specifications.

Although much of the ADAS data has been used widely and scrutinised closely, they are not error free. The user of ADAS data who discovers an error is encouraged to report it back to ADAS so that it can be corrected for all.

New releases of OPEN-ADAS will be synchronised with ADAS releases. These take place once or twice a year. A bulletin is provided on the ADAS web-site with each new release. The bulletin will include extensions to data classes and codes provided in OPEN-ADAS.

The scope of data in OPEN-ADAS is also kept under review. At appropriate times, when substantial new bodies of ADAS data of general interest are complete and verified, they will be made available in OPEN-ADAS. This includes the possibility of adding to the set of ADAS data formats currently released. User requests for release in OPEN-ADAS of further parts of the whole ADAS database will be considered.

References

Anderson H, von Hellermann M G, Hoekstra R, Horton L D, Howman A C, Konig R W T, Martin R, Olson R E and Summers H P 2000
Plasma Phys. Control. Fusion **42** 781

Badnell N R, O'Mullane M G, Summers H P, Altun Z, Bautista M A, Colgan J, Gorczyca T W, Mitnik D M, Pindzola M S and Zatsarinny O 2003
Astronomy and Astrophysics **406** 1151

Behringer K H, Summers H P, Denne B, Forrest M and Stamp M 1989
Plasma Phys. Control. Fusion **31** 2059

Summers H P, Dickson W J, O'Mullane M G, Badnell N R, Whiteford A D, Brooks D H, Lang J, Loch S D and Griffin D C 2006
Plasma Phys. Control. Fusion **48** 263

A Sample tag file

A sample .tag file is given below, the file is in XML format allowing for easy parsing by other database systems. A number of small formatting changes have been made to the file in order that it can fit withing the margins of this report. Also, only two of the transitions are listed for brevity.

```
<?xml version="1.0" encoding="UTF-8" standalone="no" ?>
<!DOCTYPE ADAS PUBLIC "-//ADAS//DTD ADAS 1.0//EN"
              "http://open.adas.ac.uk/adas.dtd">
<adf15>
        <file>
                <type>ADF15</type>
                <filename>pec96#c_pjr#c4.dat</filename>
                <directory>adf15/pec96#c</directory>
                <tagged_on>2006-07-21</tagged_on>
                <tagged_by>Allan Whiteford</tagged_by>
                <md5sum>722bda2a220dc12fe8a74c8c227bf725</md5sum>
        </file>
        <ion>
                <z0>6</z0>
                <z1>4</z1>
        </ion>
        <predecessors>
                <predecessor>
                        adf04/adas#6/mom97_ls#c4.dat
                </predecessor>
                <predecessor>
                        adf18/a17_p208/exp96#he/exp96#he_c4ls.dat
                </predecessor>
        </predecessors>
        <limits>
                <density>
                        <min units="cm-3">7.81E+05</min>
                        <max units="cm-3">7.81E+19</max>
                </density>
                <temperature>
                        <min units="eV">1.08E+00</min>
                        <max units="eV">6.46E+03</max>
                </temperature>
                <wavelength>
                        <min units="A">32.8</min>
                        <max units="A">2274.7</max>
```

```
        </wavelength>
</limits>
<contributors>
        <contributor>Martin O'Mullane</contributor>
</contributors>
<transitions>
        <transition>
                <z1>4</z1>
                <lambda units="A">40.7</lambda>
                <upper>
                        <level>3</level>
                        <cfg>1S1 2S1</cfg>
                        <m>1</m>
                        <l>0</l>
                        <j>.0</j>
                </upper>
                <lower>
                        <level>1</level>
                        <cfg>1S2</cfg>
                        <m>1</m>
                        <l>0</l>
                        <j>.0</j>
                </lower>
                <driving>
                        <level>1</level>
                        <cfg>1S2</cfg>
                        <m>1</m>
                        <l>0</l>
                        <j>.0</j>
                </driving>
                <type>Excitation</type>
        </transition>

        ... Continues at Length ...

        <transition>
                <z1>4</z1>
                <lambda units="A">2274.7</lambda>
                <upper>
                        <level>4</level>
                        <cfg>1S1 2P1</cfg>
                        <m>3</m>
                        <l>1</l>
```

```
                        <j>4.0</j>
                    </upper>
                    <lower>
                        <level>2</level>
                        <cfg>1S1 2S1</cfg>
                        <m>3</m>
                        <l>0</l>
                        <j>1.0</j>
                    </lower>
                    <type>Charge Exchange</type>
                </transition>
        </transitions>
</adf15>
```

B Database Schema

The main database schema for OPEN-ADAS is given below, the format is a MySQL dump format, small formatting changes have been made to fit inside the margins of the present report. Superfluous information has also been removed and the tables have been re-ordered to give an indication of importance and to aid in typesetting (the default of a MySQL dump is alphabetical order). Note also there is an additional database schema for OPEN-ADAS user accounts, this schema is given in appendix C.

```
-- Table structure for table `filedetail`
--

CREATE TABLE `filedetail` (
  `id` int(4) NOT NULL auto_increment,
  `filename` varchar(255) default NULL,
  `directory` varchar(255) default NULL,
  `filesize` int(4) default NULL,
  `adftype` int(2) default NULL,
  `md5sum` varchar(32) default NULL,
  `tagged_on` date default NULL,
  `tagged_by` int(2) default NULL,
  PRIMARY KEY  (`id`),
  UNIQUE KEY `id` (`id`),
  KEY `filedetail_filename` (`filename`),
  KEY `filedetail_directory` (`directory`)
);

-- Table structure for table `datatype`
--

CREATE TABLE `datatype` (
  `id` int(2) NOT NULL default '0',
  `shortdesc` varchar(8) default NULL,
  `longdesc` varchar(50) default NULL,
  PRIMARY KEY  (`id`),
  UNIQUE KEY `id` (`id`)
);
```

```
-- Table structure for table `subtype`
--

CREATE TABLE `subtype` (
  `id` int(2) NOT NULL auto_increment,
  `adftype` int(2) default NULL,
  `shortdesc` varchar(8) default NULL,
  `longdesc` varchar(40) default NULL,
  PRIMARY KEY  (`id`),
  UNIQUE KEY `id` (`id`)
);

-- Table structure for table `ion`
--

CREATE TABLE `ion` (
  `id` int(2) NOT NULL auto_increment,
  `file` int(4) default NULL,
  `z0` int(2) default NULL,
  `z` int(2) default NULL,
  `z_min` int(2) default NULL,
  `z_max` int(2) default NULL,
  PRIMARY KEY  (`id`),
  UNIQUE KEY `id` (`id`),
  KEY `ion_file` (`file`)
);

-- Table structure for table `predecessor`
--

CREATE TABLE `predecessor` (
  `id` int(4) NOT NULL auto_increment,
  `parent` int(4) default NULL,
  `child` int(4) default NULL,
  PRIMARY KEY  (`id`),
  UNIQUE KEY `id` (`id`),
  KEY `predecessor_parent` (`parent`),
  KEY `predecessor_child` (`child`)
);
```

```
-- Table structure for table ‘limits‘
--

CREATE TABLE ‘limits‘ (
  ‘id‘ int(2) NOT NULL auto_increment,
  ‘file‘ int(4) default NULL,
  ‘min_dens‘ float default NULL,
  ‘max_dens‘ float default NULL,
  ‘ref_dens‘ float default NULL,
  ‘unit_dens‘ enum(’cm-3’,’m-3’) default ’cm-3’,
  ‘min_temp‘ float default NULL,
  ‘max_temp‘ float default NULL,
  ‘ref_temp‘ float default NULL,
  ‘unit_temp‘ enum(’eV’,’K’) default ’eV’,
  ‘min_wave‘ float default NULL,
  ‘max_wave‘ float default NULL,
  ‘ref_wave‘ float default NULL,
  ‘unit_wave‘ enum(’A’,’nm’) default ’A’,
  ‘min_energy‘ float default NULL,
  ‘max_energy‘ float default NULL,
  ‘ref_energy‘ float default NULL,
  ‘unit_energy‘ enum(’eV’,’Ryd’) default ’eV’,
  ‘min_bmag‘ float default NULL,
  ‘max_bmag‘ float default NULL,
  ‘ref_bmag‘ float default NULL,
  ‘unit_bmag‘ enum(’T’) default ’T’,
  ‘min_zeff‘ float default NULL,
  ‘max_zeff‘ float default NULL,
  ‘ref_zeff‘ float default NULL,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘),
  KEY ‘limits_file‘ (‘file‘)
);

-- Table structure for table ‘people‘
--
CREATE TABLE ‘people‘ (
  ‘id‘ int(2) NOT NULL auto_increment,
  ‘fullname‘ varchar(255) default NULL,
  ‘email‘ varchar(255) default NULL,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘)
);
```

```
-- Table structure for table ‘switches‘
--

CREATE TABLE ‘switches‘ (
  ‘id‘ int(4) NOT NULL auto_increment,
  ‘file‘ int(4) default NULL,
  ‘subtype‘ int(2) default NULL,
  ‘metastable‘ int(1) default NULL,
  ‘year‘ int(2) default NULL,
  ‘ic_resolved‘ int(1) default ’0’,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘),
  KEY ‘switches_file‘ (‘file‘),
  KEY ‘switches_subtype‘ (‘subtype‘)
);

-- Table structure for table ‘beam‘
--

CREATE TABLE ‘beam‘ (
  ‘id‘ int(2) NOT NULL auto_increment,
  ‘file‘ int(4) default NULL,
  ‘z0‘ int(2) default NULL,
  ‘z‘ int(2) default NULL,
  ‘state‘ varchar(15) default NULL,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘),
  KEY ‘beam_file‘ (‘file‘)
);

-- Table structure for table ‘contributor‘
--

CREATE TABLE ‘contributor‘ (
  ‘id‘ int(2) NOT NULL auto_increment,
  ‘person‘ int(2) default NULL,
  ‘file‘ int(4) default NULL,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘),
  KEY ‘contributor_file‘ (‘file‘),
  KEY ‘contributor_person‘ (‘person‘)
);
```

```
-- Table structure for table ‘adf01_state‘
--

CREATE TABLE ‘adf01_state‘ (
  ‘id‘ int(4) NOT NULL auto_increment,
  ‘file‘ int(4) default NULL,
  ‘n‘ int(2) default NULL,
  ‘l‘ int(2) default NULL,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘),
  KEY ‘adf01_state_file‘ (‘file‘)
);


-- Table structure for table ‘adf07_transition‘
--

CREATE TABLE ‘adf07_transition‘ (
  ‘id‘ int(4) NOT NULL auto_increment,
  ‘file‘ int(4) default NULL,
  ‘isel‘ int(4) default NULL,
  ‘z‘ int(2) default NULL,
  ‘initial_cfg‘ varchar(255) default NULL,
  ‘initial_m‘ int(2) default NULL,
  ‘initial_l‘ int(2) default NULL,
  ‘final_cfg‘ varchar(255) default NULL,
  ‘final_m‘ int(2) default NULL,
  ‘final_l‘ int(2) default NULL,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘),
  KEY ‘adf07_transition_file‘ (‘file‘)
);
```

```
-- Table structure for table ‘adf04_process‘
--

CREATE TABLE ‘adf04_process‘ (
  ‘id‘ int(4) NOT NULL auto_increment,
  ‘file‘ int(4) default NULL,
  ‘excitation‘ int(1) default ’0’,
  ‘ion_impact‘ int(1) default ’0’,
  ‘recombination‘ int(1) default ’0’,
  ‘cx‘ int(1) default ’0’,
  ‘ionisation_source‘ int(1) default ’0’,
  ‘ionisation‘ int(1) default ’0’,
  ‘dr_sat‘ int(1) default ’0’,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘),
  KEY ‘adf04_process_file‘ (‘file‘)
);

-- Table structure for table ‘adf04_state‘
--

CREATE TABLE ‘adf04_state‘ (
  ‘id‘ int(4) NOT NULL auto_increment,
  ‘file‘ int(4) default NULL,
  ‘cfg‘ varchar(255) default NULL,
  ‘m‘ int(2) default NULL,
  ‘l‘ int(2) default NULL,
  ‘j‘ decimal(10,1) default NULL,
  ‘energy‘ float default NULL,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘),
  KEY ‘adf04_state_file‘ (‘file‘),
  KEY ‘adf04_state_lambda‘ (‘energy‘)
);
```

```
-- Table structure for table ‘adf08_state‘
--

CREATE TABLE ‘adf08_state‘ (
  ‘id‘ int(4) NOT NULL auto_increment,
  ‘file‘ int(4) default NULL,
  ‘idx‘ int(4) default NULL,
  ‘parent‘ int(1) default NULL,
  ‘cfg‘ varchar(255) default NULL,
  ‘m‘ int(2) default NULL,
  ‘l‘ int(2) default NULL,
  ‘j‘ decimal(10,1) default NULL,
  ‘energy‘ float default NULL,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘),
  KEY ‘adf08_state_file‘ (‘file‘),
  KEY ‘adf08_state_energy‘ (‘energy‘),
  KEY ‘adf08_state_idx‘ (‘idx‘)
);

-- Table structure for table ‘adf08_transition‘
--

CREATE TABLE ‘adf08_transition‘ (
  ‘id‘ int(4) NOT NULL auto_increment,
  ‘file‘ int(4) default NULL,
  ‘parentstate‘ int(4) default NULL,
  ‘ionstate‘ int(4) default NULL,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘),
  KEY ‘adf08_transition_file‘ (‘file‘)
);
```

```
-- Table structure for table ‘adf09_core‘
--

CREATE TABLE ‘adf09_core‘ (
  ‘id‘ int(4) NOT NULL auto_increment,
  ‘file‘ int(4) default NULL,
  ‘n_lower‘ int(2) default NULL,
  ‘n_upper‘ int(2) default NULL,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘),
  KEY ‘adf09_core_file‘ (‘file‘)
);

-- Table structure for table ‘adf09_state‘
--

CREATE TABLE ‘adf09_state‘ (
  ‘id‘ int(4) NOT NULL auto_increment,
  ‘file‘ int(4) default NULL,
  ‘parent‘ int(1) default NULL,
  ‘cfg‘ varchar(255) default NULL,
  ‘m‘ int(2) default NULL,
  ‘l‘ int(2) default NULL,
  ‘j‘ decimal(10,1) default NULL,
  ‘energy‘ float default NULL,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘),
  KEY ‘adf09_state_file‘ (‘file‘),
  KEY ‘adf09_state_energy‘ (‘energy‘)
);

-- Table structure for table ‘adf09_repn‘
--

CREATE TABLE ‘adf09_repn‘ (
  ‘id‘ int(4) NOT NULL auto_increment,
  ‘file‘ int(4) default NULL,
  ‘n‘ int(2) default NULL,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘),
  KEY ‘adf09_repn_file‘ (‘file‘)
);
```

```
-- Table structure for table ‘adf12_transition‘
--

CREATE TABLE ‘adf12_transition‘ (
  ‘id‘ int(4) NOT NULL auto_increment,
  ‘file‘ int(4) default NULL,
  ‘lambda‘ float default NULL,
  ‘upper_n‘ int(2) default NULL,
  ‘lower_n‘ int(2) default NULL,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘),
  KEY ‘adf12_transition_file‘ (‘file‘),
  KEY ‘adf12_transition_lambda‘ (‘lambda‘)
);

-- Table structure for table ‘adf13_transition‘
--

CREATE TABLE ‘adf13_transition‘ (
  ‘id‘ int(4) NOT NULL auto_increment,
  ‘file‘ int(4) default NULL,
  ‘lambda‘ float default NULL,
  ‘upper_cfg‘ varchar(255) default NULL,
  ‘upper_m‘ int(2) default NULL,
  ‘upper_l‘ int(2) default NULL,
  ‘upper_j‘ decimal(10,1) default NULL,
  ‘lower_cfg‘ varchar(255) default NULL,
  ‘lower_m‘ int(2) default NULL,
  ‘lower_l‘ int(2) default NULL,
  ‘lower_j‘ decimal(10,1) default NULL,
  ‘driving_cfg‘ varchar(255) default NULL,
  ‘driving_m‘ varchar(255) default NULL,
  ‘driving_l‘ int(2) default NULL,
  ‘driving_j‘ decimal(10,1) default NULL,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘),
  KEY ‘adf13_transition_file‘ (‘file‘),
  KEY ‘adf13_transition_lambda‘ (‘lambda‘)
);
```

```
-- Table structure for table `adf15_transition`
--

CREATE TABLE `adf15_transition` (
  `id` int(4) NOT NULL auto_increment,
  `file` int(4) default NULL,
  `lambda` float default NULL,
  `upper_cfg` varchar(255) default NULL,
  `upper_m` int(2) default NULL,
  `upper_l` int(2) default NULL,
  `upper_j` decimal(10,1) default NULL,
  `lower_cfg` varchar(255) default NULL,
  `lower_m` int(2) default NULL,
  `lower_l` int(2) default NULL,
  `lower_j` decimal(10,1) default NULL,
  `driving_cfg` varchar(255) default NULL,
  `driving_m` varchar(255) default NULL,
  `driving_l` int(2) default NULL,
  `driving_j` decimal(10,1) default NULL,
  `type` enum('Excitation','Recombination',
            'Charge Exchange','Equilibrium') default NULL,
  PRIMARY KEY  (`id`),
  UNIQUE KEY `id` (`id`),
  KEY `adf15_transition_file` (`file`),
  KEY `adf15_transition_lambda` (`lambda`)
);

-- Table structure for table `adf2122_transition`
--
CREATE TABLE `adf2122_transition` (
  `id` int(4) NOT NULL auto_increment,
  `file` int(4) default NULL,
  `lambda` float default NULL,
  `upper_cfg` varchar(255) default NULL,
  `upper_m` int(2) default NULL,
  `upper_l` int(2) default NULL,
  `lower_cfg` varchar(255) default NULL,
  `lower_m` int(2) default NULL,
  `lower_l` int(2) default NULL,
  PRIMARY KEY  (`id`),
  UNIQUE KEY `id` (`id`),
  KEY `adf2122_transition_file` (`file`)
);
```

C User Database Schema

The database schema for the user management/login system is given below, the format is a MySQL dump format, small formatting changes have been made to fit inside the margins of the present report. Superfluous information has also been removed and the tables have been re-ordered to give an indication of importance (the default of a MySQL dump is alphabetical order).

```
-- Table structure for table `user`
--
CREATE TABLE `user` (
  `id` int(4) NOT NULL auto_increment,
  `firstname` varchar(255) default NULL,
  `lastname` varchar(255) default NULL,
  `institution` varchar(255) default NULL,
  `address1` varchar(255) default NULL,
  `address2` varchar(255) default NULL,
  `address3` varchar(255) default NULL,
  `postcode` varchar(20) default NULL,
  `country` varchar(50) default NULL,
  `email` varchar(50) default NULL,
  `telephone` varchar(50) default NULL,
  `fax` varchar(50) default NULL,
  `fundamental` int(1) default NULL,
  `magnetic` int(1) default NULL,
  `inertial` int(1) default NULL,
  `astrophysics` int(1) default NULL,
  `processing` int(1) default NULL,
  `lithography` int(1) default NULL,
  `atomicdatabases` int(1) default NULL,
  `defense` int(1) default NULL,
  `otheruse` varchar(100) default NULL,
  `member` int(1) default NULL,
  `username` varchar(15) default NULL,
  `password` varchar(15) default NULL,
  `auth` int(4) default NULL,
  `startpage` varchar(255) default NULL,
  `waveunits` enum('A','nm') default NULL,
  `tempunits` enum('Default','eV','K') default NULL,
  `energyunits` enum('Default','cm-1','Ryd','eV') default NULL,
  PRIMARY KEY  (`id`),
  UNIQUE KEY `id` (`id`)
);
```

```
-- Table structure for table ‘history‘
--

CREATE TABLE ‘history‘ (
  ‘id‘ int(4) NOT NULL auto_increment,
  ‘user‘ int(4) default NULL,
  ‘type‘ int(1) default NULL,
  ‘site‘ int(1) default NULL,
  ‘text‘ blob,
  ‘file‘ varchar(255) default NULL,
  ‘time‘ datetime default NULL,
  ‘ip‘ varchar(15) default NULL,
  ‘ip_conn‘ varchar(15) default NULL,
  ‘ip_real‘ varchar(15) default NULL,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘),
  KEY ‘history_user‘ (‘user‘),
  KEY ‘history_time‘ (‘time‘),
  KEY ‘history_site‘ (‘site‘),
  KEY ‘history_type‘ (‘type‘)
);

-- Table structure for table ‘historysite‘
--

CREATE TABLE ‘historysite‘ (
  ‘id‘ int(4) NOT NULL auto_increment,
  ‘site‘ varchar(255) default NULL,
  ‘longsite‘ varchar(255) default NULL,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘)
);

-- Table structure for table ‘historytype‘
--

CREATE TABLE ‘historytype‘ (
  ‘id‘ int(4) NOT NULL auto_increment,
  ‘type‘ varchar(255) default NULL,
  ‘longtype‘ varchar(255) default NULL,
  PRIMARY KEY  (‘id‘),
  UNIQUE KEY ‘id‘ (‘id‘)
);
```

D Betatesting

The ADAS betatesting process was conducted over a number of months in the run up to the launch of the OPEN-ADAS system. It involved consultation with key experts and future users of the system. A number of invitations to beta-test were sent to members of the ADAS Project and also to people external to the ADAS Project. The list of people who responded to the beta-test are given in table 11. The definitions of the different areas of expertise are rather loose and we are simply trying to illustrate the spread of background of the beta-testers.

		Expertise							
Name	Institution	ADAS	Atomic Data	Data calculations	Fusion Diganostics	Fusion Modelling	Astrophysics	Web databases	Technical Plasmas
Nigel Badnell	Strathclyde	■	■	■			■		
Kurt Behringer	IPP-Garching	■	■	■	■	■			■
Mathias Brix	UKAEA		■		■	■			
Paul Bryans	Columbia		■	■			■		
Bob Clark	IAEA		■	■				■	
Rémy Guirlet	CEA		■		■	■		■	
Denis Humbert	IAEA		■					■	
Ratko Janev	FZ-Jülich		■	■		■		■	
Stuart Loch	Auburn	■	■	■		■	■	■	
Chris Nicholas	Strathclyde	■	■		■				
Martin O'Mullane	ADAS	■	■	■	■	■			
Thomas Pütterich	IPP-Garching	■	■	■	■	■			
Randall Smith	NASA		■	■			■	■	
Hugh Summers	ADAS	■	■	■	■	■	■		
Mike Witthoeft	NASA		■	■			■	■	

Table 11: List of people involved in OPEN-ADAS beta-testing

Appendix E is a copy of the document which was sent to the beta-testers and appendix F lists every comment received along with a response. The beta-test proved incredibly worthwhile with excellent feedback from all people concerned.

E Betatesting request

The present appendix is based on the document sent to OPEN-ADAS betatesters on the 11th of March 2008. The section headings have been modified slightly to fit the structure of the present report.

OPEN-ADAS: beta-testing guide

A D Whiteford

11th March 2008

E.1 Introduction

Thank you for taking part in the OPEN-ADAS beta-test. We appreciate you taking the time to help us in the final stages of OPEN-ADAS development.

We do not want to give too much guidance on how you should use the OPEN-ADAS site. Part of the beta-test is to ascertain how easy the site is to use in its current state and for us to address any usability deficiencies. The scope of OPEN-ADAS is discussed in subsection E.3 which should hopefully provide a sufficient background information on our main aims with the site.

However, we would like to draw attention to specific areas which we would like you to test and to give some guidance on areas where we would particularly like feedback. This is detailed in subsection E.4.

Feedback can be given in whatever way you think is appropriate, either in individual e-mails as you find problems, using the site itself to report errors or in a larger e-mail after you have finished testing — more details are given in subsection E.5. A timescale for when we would appreciate feedback is given in subsection E.2 along with the address of the OPEN-ADAS beta-test website.

E.2 Beta-test procedures

The OPEN-ADAS website for beta-testing purposes can be found at the following URL:

`http://openadas.phys.strath.ac.uk/beta`

Table 12 gives a proposed timescale to eventual deployment of OPEN-ADAS on the 6th of June 2008. Timescales are mainly chosen to give you adequate time and also to fit around the 2008 travel/work schedule of Allan Whiteford.

Date	Item
12th March 2008 – 11th April 2008	Released for beta-testing
11th April 2008	Reports from beta-testers received
14th April 2008 – 25th April 2008	Implementation of suggestions
25th April 2008	Report given back to beta-testers
28th April 2008 – 16th May 2008	Further beta-testing of bug-fixes
19th May 2008 – 23rd May 2008	Final development feedback
26th May 2008 – 30th May 2008	Visit to IAEA for final discussions
2nd June 2008 – 6th June 2008	Installation of software on live server
6th June 2008	**Site launched**
27th June 2008	Final report lodged with IAEA
October 2008	Presented to ADAS Project
Mid-late 2009	Presented to IAEA DCN
Mid-late 2009	Presented at ICAMDATA meeting

Table 12: Timescale for launch of OPEN-ADAS site.

The timeline given above is indicative of what we would like to work to but should not be regarded as definitive. As you can see after the initial beta-test which lasts for a month we will implement suggestions made and then feedback these changes for approval to the beta-testers.

As such, we would appreciate all of your comments by the 11th of April so that we can look at all of the suggestions together and take a balanced view of where our development priorities should lie. Comments after this time are also very welcome.

We, of course, welcome feedback as you test the site so please don't assume that you should only send feedback at the end of your testing or that we can't enter into dialogue during the beta-test. In particular, if you find a bug in the site which is particularly serious and is stopping you from testing then we would like to know as soon as possible.

E.3 Scope of OPEN-ADAS

The current goal of OPEN-ADAS is to allow flexible searching across a subset of the ADAS database (see table 13) which are relevant to application and access to these datasets. As such, ADAS 'driver files' are not included since they are only useful along with the associated ADAS code. Similarly, some of the more fundamental data (e.g. photo-processes) are not included but we note that they are already available and that an astrophysics-targeted initiative is in place with similar goals to OPEN-ADAS to make available such data over the web.

Class	Description	Files	Size
ADF01	charge exchange cross subsections	118	2 MB
ADF04	resolved specific ion data collections	1078	394 MB
ADF07	electron impact ionisation coefficients	67	589 kB
ADF08	radiative recombination coefficients	101	469 kB
ADF09	dielectronic recombination coefficients	1573	914 MB
ADF11	iso-nuclear master files	343	45 MB
ADF12	charge exchange effective emission coefficients	43	1 MB
ADF13	ionisation per photon coefficients	153	35 MB
ADF15	photon emissivity coefficients	174	75 MB
ADF21	effective beam stopping/excitation coefficients	218	2 MB
ADF22	effective beam emission/population coefficients	402	3 MB

Table 13: Data classes indexed and available in OPEN-ADAS.

Most of the ADAS heavy element work is also not included. This is packaged in the *superstage* framework and requires tuning to specific plasma and transport regimes. These are extensions to primarily ADF11, ADF12 and ADF15 which necessarily make the file formats more complicated. It is currently judged unsafe to give out such data without the expert guidance required to use it appropriately. After sufficient benchmarking against current experiments (this work is currently ongoing) it is feasible that such data are released with OPEN-ADAS but for the moment they are not.

OPEN-ADAS does not release any of the interactive ADAS programs and the release of subroutine libraries are limited to the relevant xxdata routines required to read the available file formats.

E.4 Searching, displaying and downloading data

E.4.1 Searching for data

There are a number of ways to search for data in OPEN-ADAS. Either by a specific data class, by wavelength, by element or freeform search.

Each specific dataclass has a custom form. We would particularly like suggestions of additions which could be made to these forms.

Searching by wavelength and by element are probably complete but we would, of course, welcome any suggestions.

The freeform search is the thing we are currently least sure about. This is designed to present a single box in the style of a modern web search (e.g. Google, Yahoo!, MSN). We have tried to anticipate what people will enter into this box but we think that this is where some of the greatest attention is required. We would encourage you to use this search facility extensively and report anything you enter which produces incomplete or unexpected matches. As part of the beta-test we will also be recording all of the searches done using the freeform search to try to understand what people would intuitively type into the box.

As examples, the following searches currently produce sensible results:

- neutral carbon influx
- 5291A or 529.1nm
- 524nm-535nm
- ArXVI or Ar15+
- xenon dielectronic recombination

the freeform search first displays best matches and then displays partial matches. Feedback would be appreciated on how useful the partial matches are. The results can also be quite lengthy, comments on whether a maximum number of results per page would be useful or simply cumbersome would also be appreciated.

We note that the freeform search can currently be quite slow, taking several seconds to display results. We can currently get around a factor of two speedup via software[12] and probably a similar factor through hardware. Limiting the results per page will also achieve a significant speedup.

[12]Changing from MySQL 4 to MySQL 5 allows more advanced queries.

E.4.2 Displaying and downloading data

On finding a file, it is possible to click on the filename and be shown information on that file. Some information is generic and other information is specific to the type of file being displayed. Feedback would be appreciated on what information should be displayed for each file class.

On the same file information screen it is possible to download the individual data file, download documentation for it or download the xxdata routines to read it. Any issues you have with downloading data would be appreciated. Some browsers assume that a file extension of `.dat` corresponds to some kind of movie and try to open the ADF file in a media player. Unfortunately there is nothing we can do about this.

Please note that whilst the individual ADAS data files contain bibliographic information in their comments this information has not been extracted into the OPEN-ADAS system. This is planned for a future development of OPEN-ADAS.

OPEN-ADAS does not currently make any attempt to display the raw data in either graphical or textual form. Whilst recommendations are welcome for improvements in this area it is likely that such improvements would happen at a later date.

E.5 Reporting errors and suggestions

E.5.1 The 'Report Error' feature

Each page has a link at the top right where you can report an error. Please feel free to use this feature if you would prefer to simply report errors and make suggestions as you find them. The 'Report Error' feature also records the page you were last looking at so if you are using this feature it should not be necessary to give a detailed explanation of the page you are visiting.

E.5.2 Alignment errors

Alignment errors or things which generally look bad can prove problematic to fix since they are a function of the computer and browser you are using. If you encounter such an error then as well as a description it would be helpful if you told us the browser (e.g. Interner Explorer, Firefox, Safari) you are using and its version (normally available in Help—About).

If you could also supply a screenshot that would be very helpful. Under Windows you can take a screenshot by pressing the 'Print Screen' (or 'Prt Sc') button on your keyboard then open up a document capable of containing graphics (e.g. MS Paint or MS Word) and simply select Edit—Paste. Under UNIX there are a number of options, we would suggest using the 'import' command. On an Apple Mac, press Cmd+Shift+4+Spacebar then point at your browser window. A file will appear on your desktop.

E.5.3 Incorrect results

Incorrect or unexpected results should not normally require a screenshot, simply a description of what you were searching for and the URL which is currently in your browser (i.e. the address at the top of the screen). Or the 'Report Error' feature can be used.

E.5.4 Internal errors

Internal errors will either manifest themself as some gibberish appearing on the screen or simply a blank screen. These are the most serious of errors. In most cases to report such an error it's only necessary to supply the URL which is currently in your browser (i.e. the address at the top of the screen) and a brief description of what you were doing. The only exception to this is when you are creating or modifying your account in which case a longer description would be helpful as the URL does not give so much information.

E.6 Things to try

As a prompt towards getting used to the system, we would welcome feedback on any difficulties you have in using the site to do the following:

- Find all the ADF04 files for neutral Helium,
- Find radiated power from charge exchange data for Carbon,
- Find DR data for Xenon,
- Find S/XB data for Beryllium between 3000 and 6000 Å,
- Find all the datafiles which have been contributed to by Allan Whiteford,
- Find beam stopping coefficients for a hydrogen beam against an argon impurity.

We hope that if the site is sufficiently intuitive then the above should be straightforward. We welcome a description of any difficulties you may have in the above and, in particular, any suggestions as to how finding the above data could be made simpler.

E.7 Conclusions

After beta-testing is completed we expect to issue a short questionnaire about how you found the site. We will try to ensure that this is not too arduous a process and will only take a few minutes of your time.

We hope that you find the site useful and come away with a positive impression that in future you would use it in addition to other searching mechanisms you may have used for ADAS data.

Finally, we thank you again for taking the time to beta-test OPEN-ADAS.

F Betatesting response

The present appendix is based on the document sent to OPEN-ADAS betatesters on the 2nd of May 2008. The section headings have been modified slightly to fit the structure of the present report.

OPEN-ADAS: initial beta-testing period

A D Whiteford

April 2008

This document lists comments received during the initial OPEN-ADAS beta-testing period and should be read in conjunction with the beta-testing instructions. Comments received by beta-testers are given in bold and the response is given below each comment or group of comments.

Comments have not been linked to specific people so that comments of a similar nature can be listed together and an aggregate response given where appropriate. Comments are mostly quoted verbatim but some have been edited slightly to fit in with the document or to provide additional context for clarity, the overall meaning of each comment has been preserved. Every comment, positive or negative, received about OPEN-ADAS is listed in this document; none have been discarded.

In addition, some freeform searchs which were performed are listed along with comments where appropriate.

F.1 General comments

"First off, kudos for a phenomenal job. The interface is easy to use and clear, and the pages are nicely clean."

"ADF15 search: it is good and flexible because not all filed have to be specified."

"The search capabilities are very good."

"Am I the first to do all tests? I think I achieved all your targets (things to try)..."

"Overall, the site is very clean and efficient. Very well done."

"I like the website."

"I have taken a look at OPEN-ADAS and submitted several error reports for your enjoyment. I will play with it again later, but it looks good. The site is very responsive and looks professional. Easy to get around as well."

The general tone of the comments received about OPEN-ADAS were positive. There was, of course, a lot of constructive criticism which was the purpose of the beta-test but all of the criticism was given in a very positive context. We are happy with the comments above and note that there are no comments whatsoever which are generally negative[13].

"In the ADAS-OPEN presentation dates I saw that a presentation of the system/database is planned for ICAMDATA 2009 meeting. However, ICAMDATA will not be held that year. Instead, ICAMDATA will be held this year, Oct. 28-31 in Beijing (see on the Web: ICAMDATA 2008).

I suggest that a presentation on ADAS-OPEN be given at the ICAMDATA 2008."

This was an error in the timetabling schedule. Attendance at ICAMDATA 2008 is unlikely due to previous commitments but not out of the question.

[13]It should be noted, however, that the majority of the beta-testers were colleagues and collaborators of Allan Whiteford.

"One of the major points to come from [a recent meeting] was that astronomers are too [busy] to collect atomic data from the literature. They are far more likely to use whatever they consider the best compilation where all data is together and in a common format. This OPEN-ADAS release may then be perfect if you are also providing routines to read the data. If you feel recognition of ADAS in the astrophysics community is important then it may be worth while trying to advertise this release to the astrophysicists."

We plan to publish OPEN-ADAS in a suitable journal and we will look at also publishing in an astrophysical oriented journal.

"I do see that I need to login to actually see the data."

"Under Search by Data class, I see that 'file details' (and presumably the data) are only accessible to registered users. Is that expected to be a feature of the actual release, i.e. you have to register to use OPEN-ADAS? That would not sit well in the astrophysics community."

This is currently under discussion and debate. The thinking was to implement a login procedure and various protections since it's easier to remove them than to build a site which is incompatible with such policies and then try to add them later.

It is likely that the final OPEN-ADAS site will be less restrictive than the current beta version in terms of mandatory logins. We are currently considering the impact of anonymous downloads on quality assurance and accountability.

F.2 Enhancement ideas

> **"Just a suggestion... maybe allow for spectroscopic notation in the charge entry."**

> **"Not obvious what to type in 'charge' box for ADF07. Is it 6, VII, +6 or 6+. Perhaps add (e.g.: 6) beside the box (given verbally)."**

The search forms for all of the data classes expected simply a number. They have been extended to allow, e.g., '+6', '6+' or VII.

> **"When [finding] all the ADF04 files for neutral Helium, [entering] element : He, he work, helium, Helium do not"**

The search forms for all of the data classes expected an element symbol or atomic number. They have been extended to also accept an element name.

> **"Also, why have two input windows when you can just have one? Have people type He0+ or HeI."**

Our feeling was that the freeform search was more suited to this kind of intuitive input and that if people are searching for a specific data class then they also want to be more prescriptive.

However, the element and charge boxes have been modified so that if someone types in something like 'He0+' or 'HeI' then the search box acts accordingly. There is purposefully no on-screen indication that this is acceptable though.

> **"Suggestion: you let people choose if they want A or nm and K or eV. How about letting people choose cm^{-1} or Ry or eV for energies?"**

This has been implemented for the listing of energy levels (we don't think it makes sense for beam energies and the like to be expressed in cm^{-1}).

> **"[When] searching by ion, is it possible to add the search criteria 'process'?"**

The ADF files effectively classify things by process or groups of processes, we've added an 'ADAS terminology' page which hopefully allows the user to better understand how to get at processes they are interested in. Extension to do a cross-database search of all fundamental data by process is something we plan to do for the next phase of OPEN-ADAS.

"Search for data in a given wavelength range : I have made a practical tool which I use when I am planning the spectrometer positions for the experiments. It draws spectral lines of a given element along a wavelength axis. Each tabulated line is represented at the corresponding wavelength by a vertical line of which the height is 1/k (k is the diffraction order), the colour corresponds to the element and the linestyle corresponds to the ionisation stage. it could be convenient for someone who is looking at a measured spectrum and wonders how to use the data in the best way. For this type of search, I have appreciated to have a more global view than in ADAS. It i easier to find data."

We are planning to implement a 'spectra search' feature which isn't nearly as advanced graphics-wise as what is described but will move in the right direction of interactively finding spectral lines in a wavelength range given some elements. However, we should note that ADAS is not trying to be a wavelength database and we'd still recommend NIST for line identification.

"Extra test: Wavelength search. Could you allow for a choice of an element and a charge? I would like it when I want to know whether a measured spectrum can be used for a given purpose (e.g. when I am preparing the spectrometer positions for an experiment)."

We think this will be covered by the addition of the 'spectra search' feature which is currently in development. It was thought that we should keep the search by wavelength and search by ion pages fairly clean and instead of trying to add to them we should make a new page designed around spectral prediction/identification. It should be noted, however, that ADAS is not trying to be a wavelength database and we still recommend NIST for such things.

The 'spectra search' page will allow for selection of multiple elements along with other parameters such as if neutral beams are present etc.

"When looking at the details of data files, it would be helpful to see the comments subsection of the data file"

A link has been added beside the 'View Origins' link which will display the comments from each file.

> **"[When finding all the ADF04 files for neutral Helium I notice that] when no box is ticked I get 20 files. When I tick only 'electron excitation' I get the same list of files. Is it logical? Maybe unimportant."**

> **"[When finding DR data for Xenon I see that] there may be something to be done about multiple choice. For example in the present case I can tick LS and IC at the same time. Does it mean 'look for both types of data' or 'look for files where both are present'?"**

The forms have been designed such that if a question is ignored completely then it will be assumed that all data is wanted in that category. This means that ticking every process box in the ADF04 entry is equivalent to ticking no boxes. Similarly for resolution in the ADF09 case. This is in keeping with not specifying a charge meaning that you want every ionisation stage. It was remarked in a previous comment that this searching mechanism was the most flexible. We think that consistency between text boxes and check boxes is important.

> **"[When finding all the ADF04 files for neutral helium] I originally checked all the 'processes' boxes and got [nothing] but figured it out and got 20 files."**

The processes box work in an 'and' fashion so if you click them all you're asking to see ADF04 files which contain every process. We think this is more useful than them being 'or'.

> **"[When finding all the datafiles which have been contributed to by Allan Whiteford I think that] a list of contributors would allow to choose easily. Maybe also a list in other fields (elements, charge states for a given element) would be useful."**

Functionallity to click on someones name in the statistics page has been added and the list of files they contributed to will be shown. This is also possible when viewing origin information in a particular file; the person's name is now clickable and will take you to the same list of files.

> **"Indicate the query at the top of the result page. For long research sessions or non expert users, it could make things easier."**

> **"Storing the last 10 queries in a scroll menu might also be useful. Saving a list of results could also help maybe."**

This is problematic to do from a technical point of view. The search-form is repeated to the user when reviewing the results but since OPEN-ADAS is a stateless implementation[14] by the time a user is looking at the details of a particular file, OPEN-ADAS has essentially 'forgot' how the user got there. The user can still use the back button but this information is stored locally in the users browser rather than on the OPEN-ADAS server.

> **"After selecting one of the search results it would be nice to have a 'back to search results' button."**

> **"Also, it would be nice to have a 'back' button (e.g. back to the ADF04 list after looking at details)."**

From a purist point of view, webpages aren't supposed to have 'back' buttons on the page. The back and forward buttons on the web browser are supposed to do this. OPEN-ADAS is fully compatible with back/forward buttons in a browser and doesn't try to maintain some sort of state — this was one of the design goals.

However, we realise that some people expect navigation inside a webpage[15]. As such we have added extra navigation buttons on the page itself. These are implemented using Javascript to simulate a press of the 'back' button.

> **"A 'To top of page' button would be convenient for long list of results."**

Similarly to the response about the 'back' button[16]. However, we realise that more and more sites are adding facilities like this and we're not trying to take some kind of puritan stance against this. Extra navigation facilities have been added similar to the 'back' buttons.

[14] This allows for bookmarking, the use of back/forward buttons in a browser and other adherence to web standards and most importantly that a user can have multiple OPEN-ADAS windows open simultaneously.

[15] It seems online shops etc. have made people understandably paranoid about pressing the 'back' button in case something is bought twice or similar.

[16] From a purist point of view webpages shouldn't provide facilities like this (e.g. on most web-browsers pressing the 'home' button on the keyboard goes to the top of the page).

"A further search within the results of an initial search would be helpful."

We agree this is a good idea but isn't fully compatible with the current structure of OPEN-ADAS. We would suggest that it's put on our medium-term development list rather than out items before launch list.

"[When finding S/XB data for Beryllium between 3000 and 6000 Å, I think] this is where a search within results would be most helpful. If I first choose Be from 'search by ion' or enter the wavelength range using 'search by wavelength' I could then refine these searches further to get what I need. However, freeform search did a good job at finding the results I wanted here."

See above. However, for this particular problem, we think that the new 'spectra search' page will help.

"[When finding DR data for Xenon I] searched for 'DR Xe' and found plenty. Not sure how many though as it doesn't tell me at the top how many results I have."

"[When finding all the datafiles which have been contributed to by Allan Whiteford I] just put your name in the freeform search and found a lot of files. I see from the stats page that there should be 147, but I'm not counting them to verify this. Wouldn't a 'number of hits' function be great."

"It would be helpful to give the number of files returned by a search at the top of the page."

"Indicating the number of results at the top and numbering the replies would be useful."

All of the search pages now have a 'Total results found: N' entry at both the top and bottom of the results list. After trying it out, we decided that numbering them individually took up too much screen space which would be better served showing additional information about the file — particularly in light of other comments that more information was needed in order to better understand what the files were.

F.3 Bugs and mistakes

> **"Also, I put in an optional use of ADAS. Is this information lost? It does not appear when I go to change my account details."**

This was a bug. Optional information is now stored.

> **"In 'Details', for some reason *Is your institution a member of the ADAS Project?* has changed from 'yes' to 'no'."**

This was a bug and has been fixed.

> **"I tried searching ADF04 and ADF09 files. The year and metastable resolution options do not seem to alter the search results."**

> **"[When finding DR data for Xenon I note that] whether I tick 'metastable resolved' or 'metastable unresolved' I get the same result. I can understand it since ADF09 is (according to official documentation) the format of resolved data. Still it is a bit confusing."**

The ADF09 form was made by cutting and pasting the ADF11 form. Of course, all ADF09 files are resolved. The underlying search didn't do anything with the selection. The option has now been removed from the form.

> **"I set my temperature preference to Kelvin and, although the given temperature range has the correct Kelvin values, the temperature label is still listed as eV."**

> **"I submitted one report saying that the temperature label for an ADF04 file was not being converted with the temperature values. Playing a little more (and with another file format), it looks like the temperature is not being converted at all. It always says the same thing regardless of the options I have set for my account."**

The temperature preference was never used throughout the site and was still an aspiration when we went to beta-test. It is now implemented.

"In the 'My Account' subsection [when] selecting 'Preferences' I chose, in 'Units', 'Angstrom', 'eV' and in 'Start Page', 'Freeform search'. I got the message: *Unknown column 'tempunits' in 'field list'*."

This was an error in moving from the development server to the betatest server and was corrected rapidly since it would have hindered betatesting. It only affected one user.

"Under preferences, I sent my preferred units to 'A'. Then when I go to 'Search by wavelength' I was asked to give wavelengths in nm. I did, asking for 1.5-1.6 nm, expecting to get some Fe^{+16} lines. However, the search used Angstroms anyway, and gave me some Fe^{+24} and Fe^{+25} lines."

"Search by wavelength: It claims to look for wavelength in nm, but it actually wants Angstroms - same for wavelength dependent data class search"

"However, I immediately stumbled over the following problem (which you may know already): when you do a search by wavelength, the program tells you to input nm but it expects and outputs Angstrom. By the way, choosing nm in the login parameters does not do anything?

I must take back my last comment to some extent. When I log in and really change my preferences to nm, everything is alright. Only if no preferences are set (if one is not logged in - or if the preferences have just never been set?), the input panel says nm and the output is in A (see attachment, not logged in). Sorry about the too fast reaction. But maybe your could change defaults consistently to nm."

There was a bug whereby when a user was not logged in the code would alternate between using a default wavelength unit of nm and A. This did not affect logged in users who had a preference set (either explicitly or implicitly). The default has been changed consistently to A. Even though the SI unit is nm we still feel that A is the spectroscopy unit most people think in — we could be convinced of course, that this is not the case.

"Statistics/List of Contributers: Elisabeth [Wolfrum] not Wolfram"

This has been fixed.

"Information on both recommended files for the 'ionisation Fe' request mentions only $Fe^0 \rightarrow Fe^+$ while files contain ionisation coefficients for all stages."

"Ionisation coefficient : the Fe recommended files show erroneous information. Only $Fe^0 \rightarrow Fe^+$ is indicated while the files contain all ionisation stages."

There was an error in the ADF07 files which meant they weren't parsed correctly by OPEN-ADAS. This has been corrected (ADAS data update D.11 in updates to the ADAS database from version 2.12).

F.4 Missing or broken links

'[When viewing [17]] None of the links on this page are working.

For example, I get the following:

The requested URL /adasman/xxdata_01.pdf was not found on this server. Apache/2.0.54 (Fedora) Server at openadas.phys.strath.ac.uk Port 80

Summarising this page and the documentation page:
`http://.../codes.php` **- codes don't download, documentation doesn't download**
`http://.../documentation.php` **- data formats links work, reading routines links do not work."**

"[When viewing [18] I] cannot download any files"

"[When finding DR data for Xenon, I notice] there is nothing under 'software libraries'."

"[When viewing [19] I] cannot download reading routine documentation"

"[When viewing [20]] the link for Software Libraries is the same as the current page with an '#' at the end. What is this supposed to go to?"

"When looking at a specific file (e.g., ls#fe16.dat), I get options to download data, documentation, and software libraries. The download data and documentation links work, but I get nothing when I hit 'Software libraries"'

"Software links don't work; I get a 404 error when asking for the ADF04 reader under 'Download code' – link goes to `http://openadas.phys.strath.ac.uk/code/xxdata_04.tar.gz`**"**

"Same is true of documentation for code — [21] goes nowhere."

[17] `http://openadas.phys.strath.ac.uk/beta/codes.php`
[18] `http://openadas.phys.strath.ac.uk/beta/codes.php`
[19] `http://openadas.phys.strath.ac.uk/beta/documentation.php`
[20] `http://openadas.phys.strath.ac.uk/beta/filedetail.php?id=70&showorigin=1`
[21] `http://openadas.phys.strath.ac.uk/adasman/xxdata_04.pdf`

"Download of code and corresponding documentation does not work 'File not found'
Documentation: code descriptions are not found... (same as above)"

At the time of going to beta-test the codes were not ready. The code will be prepared in tarfiles by the time of launch. Testing the code is seen as a separate job which requires less expertise and outside guidance so won't be circulated to beta-testers unless they specifically request to see the code in advance.

"No information yet under 'For comments and questions see: Contact Details'[22]."

We're currently unsure what to put in terms of e-mail addresses etc. It's likely we'll have a contact form for the purposes of cutting down on spam.

"Under 'Documentation', it gives a link to the entire ADAS manual[23] but it doesn't go anywhere."

This link will work when the site goes live.

"[When viewing [24]] I can't download the file; I just get a blank page when I click on the link."

The OPEN-ADAS webserver was configured to have an 8MB limit per request (the default for PHP). When pushing through this particular file it needs closer to 10MB so the server silently failed. The memory limit per request has been increased to 128MB.

[22] http://openadas.phys.strath.ac.uk/beta/contact.php
[23] http://openadas.phys.strath.ac.uk/beta/manual.php
[24] http://openadas.phys.strath.ac.uk/beta/filedetail.php?id=3741&showorigin=1

F.5 Layout and design

> **"Maybe convert Eissner form of the configurations to human-form for the level list."**

Configurations are the only part of the OPEN-ADAS underlying database which are treated as strings. As such the database has no knowledge of orbitals etc. We plan in a later release of OPEN-ADAS to address this issue. There are current ADAS plans to index and parse configurations as it will bring other benefits with regard to matching levels across files etc.

> **"I have noticed also that the transition is written differently for the 93 files and the 96 files."**

This is because we're not parsing configurations. Also 93 PEC files did not contain configuration information in them and this needs to be cross-referenced back to an ADF04 file. OPEN-ADAS currently doesn't attempt to do this but it is in our medium term plans (see response above about configurations).

> **"When giving configurations, upper case is used for l-shell rather than the lower case I would expect."**

See above for the root cause of this problem. However, we have converted all configurations to lower case on output since there is little reason for any characters in a configuration to be upper case.

> **"[When viewing [25] I note that] final period should be in <P></P> tags."**

This has been fixed.

> **"[In] the create user account form: usually * is used for required fields of a form, not optional fields; a little confusing for those who do not read the page before typing things in."**

We have swapped the use of stars so they are now next to the required parts of the personal information instead of the optional parts.

[25] `http://openadas.phys.strath.ac.uk/beta/aboutoa.php`

"[When viewing [26] you could] maybe add a link to ADAS in this page."

Done.

"Do you plan to have a news page for OPEN-ADAS? It might be nice to list changes or newly added data."

We plan for the front page of OPEN-ADAS to contain news from time to time and for new news to be displayed to users as they login.

"When it takes a while to find something, it might be nicer if something is displayed indicating that it is searching - I actually thought it wasn't working until a couple of seconds later the results appeared."

This is difficult to do using a standard browser/server setup without moving to Javascript, AJAX and all sorts of WEB2.0 things (which is technology we currently don't want to utilise with our first OPEN-ADAS release). The browser should display an egg-timer or similar. We also note that the live site will go faster than the beta-test site (which is running on a desktop PC).

"I don't know if it is intentional, but under Firefox, the label for the minimum text input field is above the field, but the label for the maximum is below the field - I think it looks weird. (Additionally, in Safari, the max label actually ends up partially on the right of the field and partially underneath it.

I have now noticed that the layout is meant to be label-field-field-label and it is a re-size issue."

This turned out to be an issue of screen size rather than browser. The horizontal field size in the wavelength search has been made smaller so that the site fits on smaller screens and windows.

[26] `http://openadas.phys.strath.ac.uk/beta/about.php`

"Under 'Search by ion', it's not clear by La and Ac are colored green and red, respectively."

We think this is the best we can do with CSS and HTML (in a finite time!). Anything more complex would required an imagemap which goes against one of our goals of making the site standards compliant and compatible with any web browser on any screen resolution.

"A comment about the display. I tend to keep my browser window on the narrow side. I noticed a couple display quirks because of this. While this can't be avoided in the extreme, the quirks seem to set in for a window size that (in my opinion) was not overly thin. The biggest culprit is the tab toolbar at the top of the 'Search by data class' window. It is not a big deal now, but if you are going to add more file types in the future, you may want to seek an alternative."

Expansion plans for OPEN-ADAS are that data classes will be split by either datatype (e.g. fundamental or derived) or by application (e.g. fusion beams or astrophysics). With the current release there aren't enough data formats to justify this splitting yet.

"For most of my testing, I used Firefox through Redhat Linux. I used Microsoft Explorer on Windows XP a little and found no big differences."

We didn't receive any browser-specific issues from anyone. We are pleased since we decided from the start to write the webpages to comply with all sorts of web standards in the hope that the site would be compatible with all browsers.

F.6 Specific data issues and the underlying ADAS framework

> **"We noticed that some state levels are strange (for example in file ls#ar4.dat). It seems that the J value is there more a statistical weight for lump levels. Is it possible to give some explanation on these levels to the user?"**

A standard convention within ADAS is for the J-value to always be $(\omega - 1)/2$. We realise this is non-standard outside of ADAS. OPEN-ADAS currently doesn't know if a file is IC or LS resolved. Future versions will detect this and suppress the printing of a dummy J value. In the meantime, the 'ADAS terminology' page should hopefully resolve some of these issues.

> **"I was interested in the C I 908.93 nm line. I was returned 6 files : 93-llu, -llr, -pju, -pjr, 96-vsu, -vsr. Where could I find the description of the difference between these files?"**

The differences are described in the ADAS manual but we realise this is rather dense. The 'u' and 'r' indicated whether the files are metastable resolved or not and the 'pj' indicates the use of projection matrices — we don't see any concise way of explaining this simply without a detailed discussion of GCR modelling which obviously can't be done inside the search results of OPEN-ADAS. We think that the 'ADAS terminology' page is the best place to cover this.

> **"[When finding all the datafiles which have been contributed to by Allan Whiteford, using] freeform search is easy. If I look for Martin's contribution, note that 'o mullane' gives only oxygen references, which is normal since 'mullane' does not give anything."**

Martin's surname is "O'Mullane" with an apostrophe as part of his name. Searching for this gives the correct behaviour. However, in recognition that this naming convention[27] is particular to Ireland (and certain parts of the USA) and is not widely used, searching for 'mullane' will now also work as a special case and find files contributed to by Martin. Searching for "o mullane" will show oxygen files contributed to by Martin as the first set of results — we think this is a reasonable compromise.

[27] We do note that Ireland was one of the first societies to adopt surnames so is well placed to set a precedent.

> **"Data are presented using the different ADAS formats. There are not very legible and I know you will provide different tools to read them. It will help to display data on screen in a more convenient way."**

Again, this is a function of the underling ADAS database but we do realise that a deficiency exists for the uninitiated. We hope that the new 'ADAS terminology' page will help with this.

On the search by wavelength page we have introduced mouse-overs so that the ADF formats are expanded for the user but there isn't enough screen space to write out the information in full on the results without dropping the transition column which we feel is the most helpful.

> **"Getting a balloon to get a short description of the different ADAS formats by dragging the mouse over the tag is a good idea."**

Mouse-overs have been used wherever we can, we hope they help with the ADAS terminology. As well as the already existing ones, many have been added as a result of the beta-testing (see above).

> **"I assume the main point of this website is to make data available to those who generally do not use ADAS. In that case, the naming convention of files isn't going to mean much to them."**

We accept this point but feel that making OPEN-ADAS a searchable framework for the underlying ADAS database is a safer route than refactoring our existing database into a completely different form. Certainly in the first stages of OPEN-ADAS.

> **"No bibliographic tracking (comment given verbally)."**

This is a feature of the underlying ADAS database. Outwith OPEN-ADAS we are currently looking at rectifying this as a general solution within ADAS via the use of the DOI system — this is labour intensive since computer readable bibliographic information is not tagged against ADAS data files. This will then be propagated through OPEN-ADAS and all publications related to a particular dataset will appear alongside its predecessors and contributors.

> **"[When finding radiated power from charge exchange data for Carbon I tried] Search by ion : 'C' produces all files for Carbon, among which I chose the ADF11 prb93_c.dat. I think I have failed this [task] since I have not found the total radiated power coefficients. But even looking at the manual it is difficult to understand the content of this file."**

It was an ADF11 PRC file which you were looking for. In 'search by ion' the text 'PRC: Charge exchange emission' should have appeared but it is in a large list. Of course, if one knows that it's an ADF11 file then going to the custom ADF11 form makes things immediately obvious (see below). We see this as a failing in the interface which we have attempted to correct by more labelling and the introduction of the ADAS terminology page.

> **"[When finding radiated power from charge exchange data for Carbon, I see that] literal search in the freeform box is no help. But found 3 files by searching within ADF11 files. Easy enough if you know ADF11 files are where to go."**

See above. We also note that the freeform search has been extended such that entering 'carbon charge exchange radiated power' (or similar) will show exactly the correct data.

> **"[When finding beam stopping coefficients for a hydrogen beam against an argon impurity I used] Search by data class : ADF22 Plasma : ar, beam : h gives file bme_99#h_ar18.dat. Straightforward."**

> **"[When finding beam stopping coefficients for a hydrogen beam against an argon impurity I] found 1 file: bms99#h_ar18.dat. Don't know if I missed any."**

The correct answer was 'bms99#h_ar18.dat'. BME files are for beam emission. We hope that the 'ADAS terminology' page will help with this.

> **"One obvious point about the data classes made available in open-adas is that the RR may not be what people are expecting in that it is not a match for the corresponding DR (ADF09) i.e. you give ADF08 and not ADF48."**

The missing ADF48 is partly historic in that the new RR files weren't in ADAS when we first started laying plans for OPEN-ADAS and also (mainly) because our derived data is still all based on ADF08. We want to be able to track ADF04 files back through the various files which contributed and this requires ADF08 files in the OPEN-ADAS system. We plan to add ADF48 files in the next phase of OPEN-ADAS.

> **"While there, I see that Mike's Fe19+ is not in OPEN-ADAS, but is in regular ADAS. Is that just a function what was set-up for beta testing?"**

> **"I noticed that you don't have my Fe19+ or F-like data there. Any plans to put it in? The Ca-like Fe paper is about to be published so that ADF04 file is available too."**

This is just a function of the version of the ADAS database that the OPEN-ADAS beta-test server was built on. OPEN-ADAS will be kept up to date with the ADAS database when it's live.

> **"It is thus difficult to determine which file has the most up-to-date data without downloading the files and looking at the comments subsection (which aren't always too helpful)."**

> **"It would be nice to rank the files by ADAS preference. Even by date generated would be a start."**

> **"When multiple files are returned for the same data, it would be good to indicate which are 'better' or more up-to-date."**

> **"The ordering of the files seems random to me though. This is a nice example of the point I made earlier about giving an indication of which files have 'best' data. (I'll leave the definition of 'best' to you.)"**

> **"By the way, my favorite keyword would be 'recommended'...."**

This is another feature of the ADAS database. A general solution is being sought which will then be pushed back into OPEN-ADAS. We note that comments can now be read without having to download the whole file first.

F.7 Freeform search

> **"Suggestion – the 'freeform search' feature is extremely nifty, and I would highlight it. Could you include that in the header so that it's in all pages, and just call it something like 'OpenADAS Freeform Search'? That way the user could easily just bail out of whatever subpage they're in to do an entirely different search. Just an idea – might misdirect some people too. Hmm."**

We've added a freeform search to the top of every page just below the options to login and manage your account. We're unsure if it will cause confusion to new users with regards to overall site navigation. We're going to put this back to the beta-testing team as a suggestion.

> **"[When finding radiated power from charge exchange data for Carbon, I see that] Freeform search : 'charge exchange' does not give anything Why?"**

> **"If I try 'whiteford charge exchange', however, I get the same results as 'whiteford'. I would expect to see the charge exchange results to come to the top."**

> **"'CX' gives some hits but 'charge exchange' doesn't. Weird."**

> **"I'm a bit helpless with the freeform search. For example: 'charge exchange' doesn't find anything. I understand it only finds what is there - so if I want a hit on 'charge exchange' it must be connected as a keyword to some data files.... So the suggestion would be such keywords for files (I know this is a lot of work)"**

> **"I also tried 'whiteford "charge exchange" ' but the page came back with 'whiteford' only in the search input with those results. Are quotes not supported (or any other operation)? I then tried charge exchange by itself and got nothing."**

This was a rather embarrassing bug: the code had '[i-1]' instead of '[$i-1]', the system was always meant to recognise the phrase 'charge exchange'.

"Some people like to call this 'charge transfer' so I would add searches for this to be directed to CX hits."

Charge transfer now also works (this was not originally implemented).

Searching for 'whiteford' works fine, as does 'whiteford ionisation' or 'whiteford ionization' (good job ;)).

We've tried wherever possible to allow for multiple spellings of the same thing. The best example is 'ionization' and 'ionisation' but element names (e.g. 'aluminium' and 'aluminum' plus others) are also supported.

"'dielectronic' gives nothing but 'dielectronic recombination' and 'DR' works fine. I would expect 'dielectronic' to be an okay short-cut."

'dielectronic' is now a short-cut.

"We noticed using the free form that 'C 2+' doesn't work, while c iii or c2+ or c+2 does."

'C 2+' and 'C +2' now work.

"[When doing a] freeform search : 'radiated power carbon' produces the less relevant electron impact ionisation coefficients, CX cross subsections etc. before CX effective emission coefficients. The score is identical for all replies."

The system didn't understand the term 'radiated power' at all so the result was just for carbon. The system now understands 'radiated', 'power' and 'radiation'.

"Freeform search : 'charge exchange emission carbon' produces a useless element column while 'charge exchange emission' (without element) does not; Add an element column when element is not prescribed?"

An element column has been added in place of the score column. Unfortunately it's present all the time. Because the system presents alternative elements in the 'partial' results subsection it's necessary for layout purposes for the element to be printed everywhere.

"What is the meaning of the score?"

It's an internal number and is only displayed for testing purposes. The final site will not display a score, an ion specification will be displayed here instead — see above. The exact algorithm used is fairly complex but will be documented in the final report for this phase of OPEN-ADAS.

"I did a search for ADF04, ADF09, ADF15 etc. nothing is listed in the 'Reasons' column."

This was because the filetype was implicitly listed in the 'type of data' column. In retrospect this will clearly cause confusion and a reason is now printed.

"After the first search, we obtain a list of files satisfying the request. Is it possible to have on that page more information regarding the file than the format and name of the file which is not very useful? Production date, contributor, data description (contents may be too long)."

It's difficult to judge exactly what the user will be looking for from the context of the search alone. We note the type of data and the reasons it's selected should now be more transparent (see above) comment. We also note that an ion column is printed where its deemed appropriate (also see above).

"[Freeform search] breaks when I put 2 spaces in search field."

Multiple spaces are now treated equally to one space.

"'Ni electron impact ionisation' also gives some DR results."

There are no electron impact ionisation coefficients (i.e. ADF07 files) for Ni. Hence the system responds by just suggesting some Ni data and then some EEI data. The 'Ni' data are suggested first because 'Ni' was the first search term.

"'EII' is not recognised as abbreviation of 'electron impact ionisation'."

It is now recognised.

"Can you implement the '-' character that Google uses to perform searches where the following word does not appear?"

We think this is a fantastic idea but it would require re-factoring the freeform search. We think it's dangerous to make such a big change between beta-testing and putting the site live. We hope to implement this in the future.

"Not sure if I sent a specific e-mail, but searching for ion charge q+ fails, but +q or q works. Even more curious since ions are displayed as X^{q+} !"

It was more luck than judgment that '+q' worked (some underlying code treats, e.g., '+3' is a number to provide symmetry with '-3' being a number). Code is now explicitly in place to handle both the '+q' and 'q+' cases.

F.8 List of freeform searches

As part of the beta-test, every freeform search was recorded. Ones which would have produced poor results are listed here and comments given. Freeform searches which were already handled sensibly by OPEN-ADAS have been discarded from this subsection.

- `Ar +1 electron impact ionisation`
- `Ar +1 electron ionisation`
- `Ar +2`
- `Ar 2`
- `Ar 2+`
- `Ar III excitation`
- `Ar iii`
- `C +5`
- `C VI`
- `Carbon IV ionization`
- `Fe`
- `Fe XVII`
- `Fe XVII collision`
- `Fe XVIII`
- `Fe XX`
- `Fe XXX`
- `n 0`
- `n i`

These searches would not have worked because it was assumed that the charge had to be next the element (e.g. 'c2+' worked but 'c 2+') didn't. This has been corrected.

- `H(+) - H charge exchange`
- `He H cross subsection`
- `He(2+) + H charge exchange`
- `c charge exchange`
- `c charge transfer`
- `charge exchange`
- `charge exchange carbon`
- `charge exchange emission`
- `charge exchange emission C`
- `charge exchange emission carbon`
- `charge exchange fe`
- `charge transfer`
- `h beam ar Charge Exchange Cross subsections`
- `hydrogen beam argon Charge Exchange Cross subsections`
- `whiteford "charge exchange"`
- `whiteford charge exchange`
- `beam h ar Charge Exchange Cross subsections`

These didn't work because 'charge exchange' wasn't recognised due to a bug. The will now work. Charge transfer is also now recognised.

- `CER`
- `CT`

We don't know what these searches are trying to find. CT could be carbon-tritium molecule and CER is a spectrometer system at AUG. Both our outside the scope of OPEN-ADAS.

- `Ar+ 2`

This will still not work but presumably was only entered after 'Ar 2+' didn't work.

- `I`
- `V I`

We're not sure what was being searched for here.

- `fitting`
- `spectral fitting`

Supplying codes for spectral fitting is outside the scope of OPEN-ADAS so nothing is returned.

- `a.  d.  whiteford`
- `a.d.  whiteford`
- `allan`
- `allan d whiteford`
- `allan whiteford`

All of these work although the "a.d." etc. aren't necessary.

- `a.d.whiteford`

This didn't work and still doesn't due to the parsing algorithm.

- `ar  xvi`
- `ar   xvi`

These caused problems because of multiple spaces, this has been corrected.

- `eii`
- `eii fe`

EII wasn't reconginsed, it is now.

- `equilibrium`
- `ionisation equilibrium`

'Equilibrium' isn't recocognised since none of the ADAS data assume ionisation equilbrium.

- `escape`

This may be looking for escape factors, nothing is returned.

- `line`
- `line radiation`
- `radiated power`
- `radiated power carbon`
- `radiated power carbon`
- `radiated power charge exchange`
- `radiated power from charge exchange for C`
- `radiative power from charge exchange for C`

These didn't work previously, they do now.

- `o mullane`

This didn't work previously, it does now.

F.9 Summary

We think that the OPEN-ADAS beta-test has been an extremely positive process. All of the beta-testers were broadly enthusiastic about OPEN-ADAS and its implementation; the various criticisms were all constructive.

The site design and usability was very well received and has been tested on Windows, Linux and Mac using a combination of Internet Explorer, Firefox and Safari. No browser specific issues were reported.

Many comments were made which are relevant to the underlying ADAS database as much as they are to OPEN-ADAS. Many of these revolved around naming conventions and specific ADAS terminology. In light of these comments we have created an 'ADAS terminology' page to help with confusion. Others were associated with identifying the best available data which is something which is currently being considered by the ADAS Project and which will feed into OPEN-ADAS. Similarly with the lack of computer-parsable bibliographic tracking.

A number of software bugs were found; these were all minor in nature and all of them have been corrected. Most enhancement suggestions have been implemented or reasons given for non-implementation.

The issue of mandatory logins was raised which is something that will be considered in the run up to the launch of OPEN-ADAS.

The freeform search feature was positively received and as a result of a comment made has been added to the header of every page. We seek opinions as to whether this will add functionallity or add to navigation confusion. The capabilities of freeform searching were improved as part of the beta-test when looking at specific searches and the terms people were using. We are increasingly confident that the freeform search facility will be a success.

Overall, the development of OPEN-ADAS has benefited greatly from beta-testing and we consider it a very well suited release model for future enhancements to the site.

G Terms and conditions

Use of the OPEN-ADAS system comes with some terms and conditions. The terms and conditions of OPEN-ADAS v1.0 are given below.

> **The user of the OPEN-ADAS system and data (hereinafter "the User") accepts the following terms and conditions:**
>
> 1. **The University of Strathclyde uses all reasonable endeavours to ensure the accuracy of the data provided and any information given, but the University makes no warranty, expressed or implied as to its accuracy, integrity, fitness for purpose and shall not be responsible for the use to which the data is put by the User and/or any consequences arising out of any inaccuracies or omissions.**
> 2. **Any downloaded OPEN-ADAS file is made available here for the personal use of the User only. It must not be used for any commercial application, incorporated into any web site or in any form re-distributed without express prior written permission from the ADAS Project. In particular, but not by way of limitation, it must not be:**
>   - **inserted into a managed database structure**
>   - **redistributed along with a modelling or analysis code**
>   - **made available on a public website.**
>
> **Permission for OPEN-ADAS data incorporation in non-commercial code/system development for scientific advance will not be unreasonably withheld, but will be subject to written agreement on a case by case basis.**
>
> **The User will indemnify the University of Strathclyde and keep it fully and effectively indemnified against each and every claim made against the University as a result of the User's use of the data.**

These terms are not designed to restrict people using ADAS data in their analysis but do place some restrictions on redistribution of the downloaded data.

H Example source code

Each of the ADAS subroutines released with OPEN-ADAS as detailed in section 5 come with a small example/test program to illustrate their use. Below is an example of the code which comes with the `xxdata_04` subroutine. The example code opens a file for reading and then passes the unit to `xxdata_04` which reads the file. The routine then prints a data to the screen.

```
       PROGRAM TEST

       IMPLICIT NONE
C-----------------------------------------------------------------------
C  Purpose:
C          Test the XXDATA_04 routine and also provide a brief
C          example of its use.
C
C  Explanaton:
C          This program is distributed as part of the ADAS
C          subroutine library either via direct CVS to ADAS Project
C          members or via download by OPEN-ADAS users. It reads a
C          file called "test.dat" (distributed along with this
C          program) and prints out some of the contents. The
C          program is intended to serve as an example of using the
C          XXDATA_04 subroutine as well as testing it. A short
C          shell script called "test.sh" is used to compile and
C          test the code.
C
C  Variables:
C          All variables are documented by XXDATA_04. See either the
C          Fortran source or the PDF documentation for the routine.
C          Variables not passed into XXDATA_04 are trivial in nature.
C
C  Routines:
C          Routine    Source    Brief description
C          ------------------------------------------------------------
C          XXDATA_04  ADAS      Read complete data from an ADF04 file
C
C  Author : Allan Whiteford
C
C  Date   : 11/01/08
C
c-----------------------------------------------------------------------
```

```
C-----------------------------------------------------------------------
C     Parameters required by XXDATA_04
C     --------------------------------
      INTEGER   NVMAX      , NDLEV
      INTEGER   NDTRN      , NDQDN
      INTEGER   NDMET
      PARAMETER( NVMAX = 14   , NDLEV= 200,
     &           NDTRN = 5000 , NDQDN = 6   , NDMET=5)
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
C     Input variables (i.e. non-parameter) required by XXDATA_04
C     ----------------------------------------------------------
      INTEGER   IUNIT           , ITIEACTN
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
C     Output variables required by XXDATA_04
C     --------------------------------------
      INTEGER   IORB          ,
     &          IL            ,
     &          IZ            , IZ0         , IZ1     ,
     &          NV            , ITRAN       ,
     &          MAXLEV        , NPL         , IADFTYP
      INTEGER   I1A(NDTRN)  , I2A(NDTRN)
      INTEGER   IA(NDLEV)     , ISA(NDLEV)    , ILA(NDLEV)
      INTEGER   IPLA(NDMET,NDLEV)             , NPLA(NDLEV)
      REAL*8    BWNO    , BWNOA(NDMET)    , PRTWTA(NDMET)
      REAL*8    ZPLA(NDMET,NDLEV)
      REAL*8    SCEF(NVMAX)
      REAL*8    XJA(NDLEV)  , WA(NDLEV)
      REAL*8    AVAL(NDTRN) , SCOM(NVMAX,NDTRN) , BETH(NDTRN)
      REAL*8    QDORB((NDQDN*(NDQDN+1))/2) , QDN(NDQDN)
      CHARACTER CPLA(NDLEV)*1 , CPRTA(NDMET)*9   , TCODE(NDTRN)*1
      CHARACTER TITLED*3      , CSTRGA(NDLEV)*18
      LOGICAL   LPRN        , LCPL            , LORB       , LBETH
      LOGICAL   LETYP       , LPTYP           , LRTYP      , LHTYP   ,
     &          LITYP       , LSTYP           , LLTYP
      LOGICAL   LTIED(NDLEV),LBSETA(NDMET)
      LOGICAL   LQDORB((NDQDN*(NDQDN+1))/2)
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
C     Variables only used by this test program
C     ----------------------------------------
      CHARACTER*80 DSNIN
      INTEGER   I             , IPL
C-----------------------------------------------------------------------
```

```
C-----------------------------------------------------------------------
C     Open input file for reading and set option to not stop when
C     encountering untied levels.
C     --------------------------
      IUNIT = 10
      DSNIN= 'test.dat'
      OPEN(UNIT = IUNIT , FILE=DSNIN , STATUS = 'OLD')
      ITIEACTN=1
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
C     Pass unit number and dimension parameters to XXDATA_01 and
C     get back contents of file.
C     --------------------------

      CALL XXDATA_04( IUNIT  ,
     &                NDLEV  , NDTRN  , NDMET , NDQDN , NVMAX ,
     &                TITLED , IZ     , IZ0   , IZ1   , BWNO  ,
     &                NPL    , BWNOA  , LBSETA, PRTWTA, CPRTA ,
     &                IL     , QDORB  , LQDORB, QDN   , IORB  ,
     &                IA     , CSTRGA , ISA   , ILA   , XJA   ,
     &                WA     ,
     &                CPLA   , NPLA   , IPLA  , ZPLA  ,
     &                NV     , SCEF   ,
     &                ITRAN  , MAXLEV ,
     &                TCODE  , I1A    , I2A   , AVAL  , SCOM  ,
     &                BETH   ,
     &                IADFTYP, LPRN   , LCPL  , LORB , LBETH ,
     &                LETYP  , LPTYP  , LRTYP  , LHTYP, LITYP ,
     &                LSTYP  , LLTYP  , ITIEACTN, LTIED
     &              )
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
C     Print out some of the contents to screen
C     ----------------------------------------

      PRINT *,'XXDATA_04 Test Program'
      PRINT *,'----------------------'
      PRINT *,' '
      PRINT *,'The following is some information about the'
      PRINT *,'input file: '//DSNIN
      PRINT *,' '
      PRINT *,'NDLEV  , NDTRN  , NDMET , NDQDN , NVMAX=',
     &                   NDLEV  , NDTRN  , NDMET , NDQDN , NVMAX
      PRINT *,' '
      PRINT *,'TITLED,IZ,IZ0,IZ1,BWNO=',
     &                   TITLED,IZ,IZ0,IZ1,BWNO
      PRINT *,' '
```

```
 PRINT *, 'NPL=',NPL
 IF(NPL.GT.0) THEN
     PRINT *,'IPL        BWNOA     LBSETA  PRTWTA   CPRTA'
     DO IPL=1,NPL
       PRINT '(I4,2X,F15.1,3X,L1,2X,F8.3,4X,1A9)',
&        IPL, BWNOA(IPL), LBSETA(IPL), PRTWTA(IPL), CPRTA(IPL)
     ENDDO
 ENDIF
 PRINT *,' '
 PRINT *,'IL,NV,ITRAN=',IL,NV,ITRAN
 PRINT *,' '
 PRINT *, 'IORB=',IORB
 IF(IORB.GT.0) THEN
     PRINT *,'IORB         QDORB   LQDORB    QDN'
     DO I=1,IORB
       PRINT '(I4,2X,F15.8,3X,L1,2X,F10.5)',
&        I, QDORB(I), LQDORB(I), QDN(I)
     ENDDO
 ENDIF

 PRINT *,' '
 PRINT *,'Check print for levels 1 and IL :-'
 PRINT *,IA(1),' ',CSTRGA(1),ISA(1),ILA(1),XJA(1),
&                  WA(1)
 PRINT *,IA(IL),' ',CSTRGA(IL),ISA(IL),ILA(IL),XJA(IL),
&                  WA(IL)

 PRINT *,' '

 PRINT *,'Check parent links for levels 1 and IL :-'
 PRINT *,'CPLA=',(CPLA(I),I=1,IL)
 PRINT *,'NPLA=',(NPLA(I),I=1,IL)
 PRINT *,'IA(1),NPLA(1),CPLA(1)=',IA(1),NPLA(1),'  ',
&                   CPLA(1)
 PRINT *,'  IPLA(1,1),ZPLA(1,1)=',
&                     IPLA(1,1),ZPLA(1,1)
 PRINT *,'IA(IL),NPLA(IL),CPLA(IL)=',IA(IL),NPLA(IL),
&                    '  ',CPLA(IL)
 PRINT *,'  IPLA(NPLA(IL),IL),ZPLA(NPLA(IL),IL)=',
&                     IPLA(NPLA(IL),IL),ZPLA(NPLA(IL),IL)
```

```
      PRINT *,' '
      PRINT *,'Check print for temperatures 1 and NV :-'
      PRINT '(1P,2D10.2)',SCEF(1),SCEF(NV)
      PRINT *,' '
      PRINT *,'CHECK PRINT FOR TRNS. 1,1 AND NV,ITRAN,:-'
      PRINT '(A1,2I5,1P3D10.2)',
     &                  TCODE(1),I2A(1),I1A(1),AVAL(1),SCOM(1,1),
     &                  SCOM(NV,1)
      PRINT '(A1,2I5,1P3D10.2)',
     &                  TCODE(ITRAN),I2A(ITRAN),I1A(ITRAN),
     &                  AVAL(ITRAN),SCOM(1,ITRAN),SCOM(NV,ITRAN)
      PRINT *,' '
      PRINT *,'IADFTYP=',IADFTYP
      PRINT *,' '
      PRINT *,'LPRN, LCPL, LORB,LBETH=',
     &                   LPRN, LCPL, LORB, LBETH
      PRINT *,'LETYP, LPTYP, LRTYP, LHTYP, LITYP=',
     &                   LETYP, LPTYP, LRTYP, LHTYP, LITYP
      PRINT *,'LSTYP, LLTYP=',
     &                   LSTYP, LLTYP
C-----------------------------------------------------------------------
       END
```

OPEN-ADAS

—

The first twelve months

Allan Whiteford, Martin O'Mullane and Hugh Summers

7th September 2009

IAEA DCN Meeting, 07/09/09

OPEN-ADAS

—

The first twelve months

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IAEA DCN Meeting, 07/09/09

Overview of ADAS

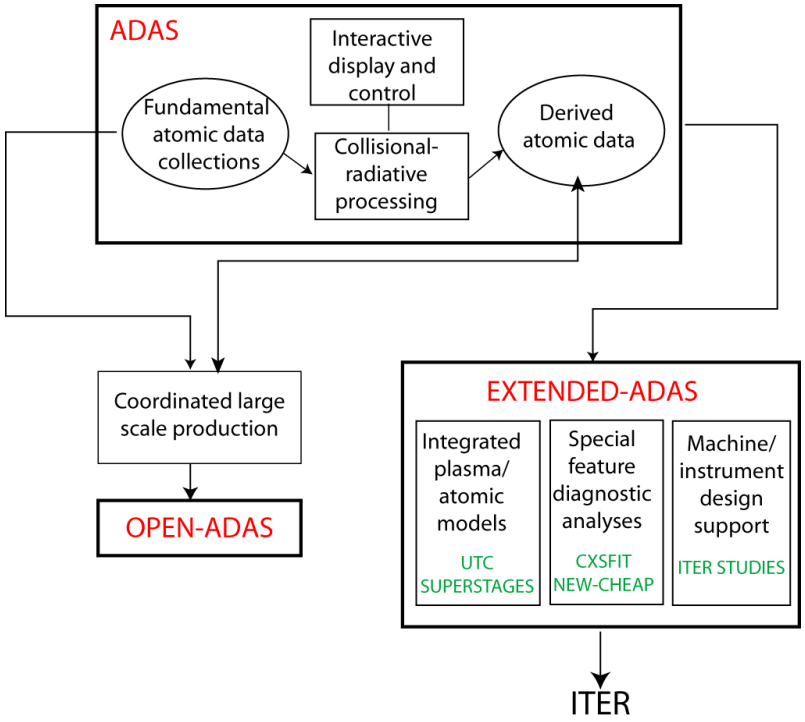
- The ADAS Project is a self-funding (i.e. funded by participants) project consisting of most major fusion laboratories along with other astrophysical and university groups. In its present incarnation it is over ten years old but the roots in JET go back twenty years.

- As an implementation, it is an interconnected set of computer codes and data collections for modelling the radiating properties of ions and atoms in plasmas.

- Historical roots are in fusion (JET) and so are the bulk of the users/members. Has also been extensively applied to astrophysics.

- Is governed by a steering committee coming from its members. Day to day running and implementation is done by the University of Strathclyde.

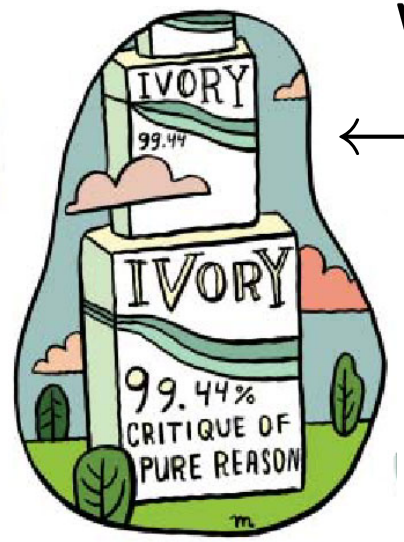
Schematic of ADAS Organisation



Size and Scope of use

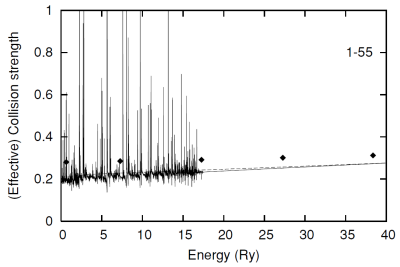
- Rough idea of the computational 'size' of ADAS:
  - 3.0GB of data in 20,103 distinct files,
  - 425,253 lines of Fortran and 406,225 lines of IDL,
  - also contains C, Perl, csh, Matlab and C++ code,
  - tentative plans to expand to support Python.
- Used extensively in spectroscopic fusion diagnostic analysis.
- Integrated into key fusion transport codes
  - e.g. Strahl, JETTO, SANCO, CHEAP, EDGE2D, B2-IRENE, ERO etc.
- The Project currently has 28 members across the world.

What does ADAS do?

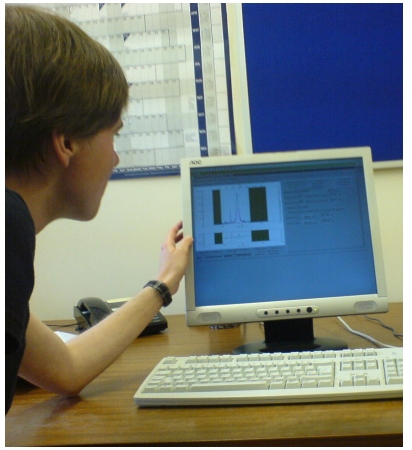


← Universities

Fusion labs →



← ADAS →
understands both of these groups!



Yes, but what does it actually do?

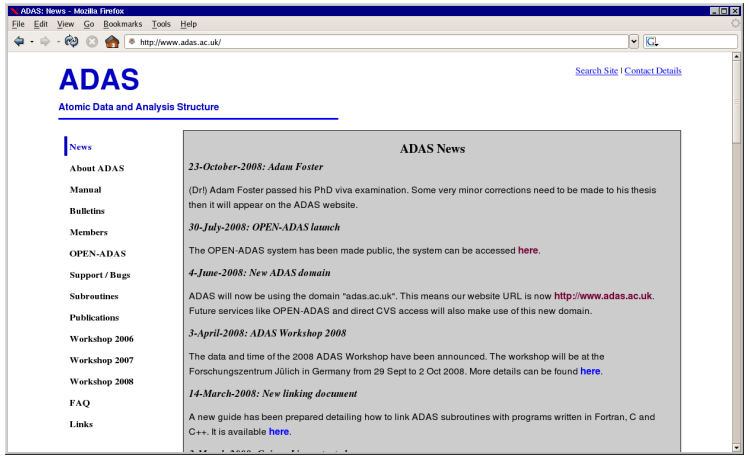
- ADAS, as a computer system, is designed to:
  - provide codes which are easy to use,
  - provide subroutine libraries for inclusion in other codes,
  - allow direct access to diagnostically relevant data.

- ADAS, as an organisation:
  - provides guidance (training courses, visits etc.) on running codes,
  - gives recommendation on the best data to use,
  - assists in analysis and development of analysis tools and models.

ADAS brings people (diagnosticians, modellers and atomic physicists) together on the topic of atomic physics for magnetically confined fusion.

Parts of ADAS

- Interactive ADAS
- The ADAS database
- Extended ADAS
- ADAS subroutine library
- ADAS Documentation (over 4000 pages!)
- Extended ADAS
- **OPEN-ADAS**



http://www.adas.ac.uk

OPEN-ADAS

- OPEN-ADAS is a joint development between the IAEA and the ADAS Project.
- Main goals are:
  - to index the data contained within the ADAS database,
  - to provide a searching system for these data,
  - to re-work the documentation and data status,
  - to provide access to the data freely via the web.
- With the exception of the last point, all of the above have benefit to ADAS Project members.
- Primary goal, from the point of view of non-ADAS members is to disseminate key data to a wider user base.

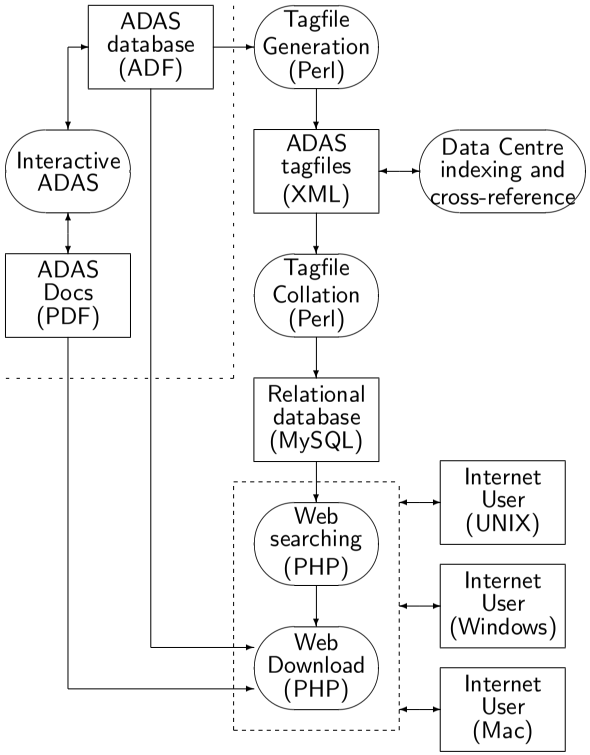
Scope of OPEN-ADAS

- OPEN-ADAS is limited to a selection of key data classes:
  - key diagnostic data classes for fusion are targeted,
  - opacity (and related data) already available,
  - no point in releasing driver files.
- OPEN-ADAS will not release any of the ADAS code, only data,
  - exception is code necessary for reading the data.
- New developments with flexible partitioning will not be included:
  - still in development,
  - need to be tuned to transport characteristics etc.,
  - best used with close support from ADAS personnel.

OPEN-ADAS data classes

Class	Description	Files	Size
ADF01	Charge exchange cross sections	118	1.9 MB
ADF04	Resolved specific ion data collections	1132	464 MB
ADF07	Electron impact ionisation coefficients	67	0.6 MB
ADF08	Radiative recombination coefficients	100	0.5 MB
ADF09	Dielectronic recombination coefficients	1619	1.1 GB
ADF11	Iso-nuclear master files	352	45.4 MB
ADF12	Charge exchange emission coefficients	43	1.1 MB
ADF13	Ionisation per photon coefficients	153	35.2 MB
ADF15	Photon emissivity coefficients	176	74.5 MB
ADF21	Effective beam stopping coefficients	218	1.8 MB
ADF22	Effective beam emission coefficients	402	3.4 MB
	Total	4380	1.71 GB

Implementation



The first twelve months

- OPEN-ADAS was launched at the end of July 2009.
- Statistics in this talk are based from 1st August 2008 – 1st August 2009.
- Since launch almost 100% server uptime (two power cuts).
- Some feedback but no complaints or bugs with the system.
- Seemless upgrade from ADAS Database v2.12 to v2.13 in October 2008.

Search Engine* Ranking

Term	Reason	Pos.
open-adas	User has heard of OPEN-ADAS	1
open adas	User has heard of OPEN-ADAS	1
adas	User has heard of ADAS	15
adas atomic	'ADAS' wasn't on first page of results	1
adas fusion	'ADAS' wasn't on first page of results	1
adf04	User has heard of ADF04 files	18
adf11	User has heard of ADF11 files	13
adf01	User has heard of ADF01 files	14
pec96#h_pju#h0.dat	User has file but isn't sure what it is	1
nrb00#he_xe52icr13.dat	User has file but isn't sure what it is	1
flike_mcw05#fe17.dat	User has file but isn't sure what it is	1
atomic data	General search for atomic data	40
atomic data fusion	General search for atomic data	41

* http://www.google.ca was used so as not to bias UK based results.

Signups

- In order to download data, (free) registration is required.
- As of 1st August 2009 (twelve months since launch):
  - 124 registered users,
  - 35 from ADAS member institutions,
  - 89 from non-ADAS member institutions.
- Following statistical breakdowns are based on above but as of Friday there had been an additional eleven registrations.

Countries

Country	Number of users	Country	Number of users
Australia	1	Not Specified	2
Austria	2	Northern Ireland	2
Belgium	1	Pakistan	1
Canada	2	Poland	1
China	6	Portugal	1
Egypt	1	Romania	2
England	1	Russia	3
France	6	Scotland	2
Germany	18	Slovenia	1
India	6	Spain	6
Italy	2	Sweden	1
Japan	4	Switzerland	4
Korea	1	Tunisia	1
Latvia	2	UK	7
Lithuania	1	Ukraine	1
Mexico	1	USA	34

Signups per month

Month	Number of Signups
Betatest	12
August 2008	5
September 2008	11
October 2008	18
November 2008	8
December 2008	5
January 2008	9
February 2008	6
March 2009	11
April 2009	5
May 2009	16
June 2009	11
July 2009	7

User Interests

Interest	Number* of interested users
Fundamental Atomic Physics	60
Magnetically Confined Fusion	69
Inertially Confined Fusion	11
Astrophysics	32
Plasma Processing	40
Lithography	0
Atomic Databases	68
Defence	2
Other	0

* Note: users can specify as many interests as they like.

Searching Mechanisms

Searching Mechanism	Number of Uses
Freeform searching	527
Wavelength searching	236
Per-ion Searching	1434*
ADF01 Specific Search	256
ADF04 Specific Search	260
ADF07 Specific Search	143
ADF08 Specific Search	115
ADF09 Specific Search	37
ADF11 Specific Search	72
ADF12 Specific Search	84
ADF13 Specific Search	63
ADF15 Specific Search	123
ADF20 Specific Search	0
ADF21 Specific Search	41

*Note: per-ion searching is only an estimate.

Views and downloads

Type of file	Number of Views*	Number of Downloads
ADF01	117	47
ADF04	354	125
ADF07	93	49
ADF08	72	23
ADF09	49	9
ADF11	234	137
ADF12	68	28
ADF13	54	17
ADF15	198	82
ADF21	32	10
ADF22	27	15
Total	1298	542

* Note: only counting views of registered users, unregistered users and search engines make up the vast majority of the number of views. Only registered users can download data.

Did OPEN-ADAS meet expectations?

- Around 70% of users are from non-ADAS member institutions.
- Good geographical spread of users.
- Steady stream of people registering with the site.
- User interest is focussed on atomic physics, databases and fusion.
- Freeform search is well used.
- Fundamental data in ADF04 files is being distributed more widely.
- Derived data, especially ADF11 and ADF15 are being downloaded.

Conclusions

- Talk covered:
  - background aspects of ADAS,
  - scope and design of OPEN-ADAS,
  - usage of OPEN-ADAS in the first twelve months.

- The ADAS database is not the only part of ADAS but it is arguably the most important and certainly core to everything which ADAS does. OPEN-ADAS is allowing free access to this database.

- We think that our database complements rather than competes with other atomic physics databases.

- As such, ADAS would like to join the DCN as an official member.