

OPEN-ADAS and data integrity



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

Allan Whiteford, Martin O'Mullane and Hugh Summers

with special thanks to:

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.

1st October 2008

ADAS Workshop, September/October 2008

Contents

- Background.
- Data classes covered by OPEN-ADAS.
- Downloadable code.
- Web interface.
- 'Data integrity'
- Usage so far.
- Conclusions.

Background

- OPEN-ADAS is a joint development between the IAEA and the ADAS Project.
- Successfully launched at the end of July 2008.
- 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

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 formats

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

Downloadable code example

File	Contents/Purpose
README	File explaining contents of each file
LICENSE	License information
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
test.sh	Test script to compile and run test.for
test.dat	Test ADF04 file for test.for to read

Web Interface

- Web interface written in PHP and outputs XHTML.
- Allows interactive searching of the database via a number of routes:
 - searching by data class,
 - cross-data class searching by ion,
 - cross-data searching by wavelength,
 - general free-form search.
- Gives information on contents of each data file.
- Option to download the file, reading routines or documentation.

Freeform searching

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

Some pictures...

OPEN-ADAS

Atomic Data and Analysis Structure

OPEN-ADAS Version 1.0

[Report Error](#) | [My Account](#) | [Log Out](#)

Freeform search

Search by wavelength

Search by ion

Search by data class

Documentation

Download code

Terminology

Statistics

About ADAS

About OPEN-ADAS

ADF01	ADF04	ADF07	ADF08	ADF09	ADF11	ADF12	ADF13	ADF15	ADF21	ADF22
-------	-------	-------	-------	-------	-------	-------	-------	--------------	-------	-------

Search ADF15 Files

Photon Emissivity Coefficients

<p>Wavelength</p> <p>Minimum (Å) <input style="width: 100%;" type="text"/></p> <p>Maximum (Å) <input style="width: 100%;" type="text"/></p>	<p>Ion</p> <p>Element <input style="width: 100%;" type="text"/></p> <p>Charge <input style="width: 100%;" type="text"/></p>
--	--

Resolve Results By

Transition (longer list)
 File (shorter list)

For comments and questions see: [Contact Details](#)

© Copyright 1995-2008 The ADAS Project

- [Search by data class](#)
- [Documentation](#)
- [Download code](#)
- [Terminology](#)
- [Statistics](#)
- [About ADAS](#)
- [About OPEN-ADAS](#)

Wavelength		Ion	
Minimum (Å)	<input type="text" value="4000"/>	Element	<input type="text" value="c"/>
Maximum (Å)	<input type="text" value="5000"/>	Charge	<input type="text"/>

Resolve Results By

Transition (longer list)
 File (shorter list)

Total results found: 41

Wavelength	Ion	Transition	File Details
4159.9Å	C ²⁺	2s1 5f1 ³ F _{10,0} → 2p1 3p1 ³ D _{7,0}	pec96#c_vsr#c2.dat
4159.9Å	C ²⁺	2s1 5f1 ³ F _{10,0} → 2p1 3p1 ³ D _{7,0}	pec96#c_vsu#c2.dat
4237.6Å	C ²⁺	2p1 3d1 ¹ P _{1,0} → 2p1 3p1 ³ D _{7,0}	pec96#c_vsr#c2.dat
4237.6Å	C ²⁺	2p1 3d1 ¹ P _{1,0} → 2p1 3p1 ³ D _{7,0}	pec96#c_vsu#c2.dat
4248.5Å	C ²⁺	2s1 5p1 ¹ P _{1,0} → 2p1 3p1 ¹ P _{1,0}	pec96#c_vsr#c2.dat
4248.5Å	C ²⁺	2s1 5p1 ¹ P _{1,0} → 2p1 3p1 ¹ P _{1,0}	pec96#c_vsu#c2.dat
4268.3Å	C ⁺	2s2 4f1 ² F _{6,5} → 2s2 3d1 ² D _{4,5}	pec96#c_vsr#c1.dat
4268.3Å	C ⁺	2s2 4f1 ² F _{6,5} → 2s2 3d1 ² D _{4,5}	pec96#c_vsu#c1.dat
4326.8Å	C ²⁺	2p1 3p1 ¹ D _{2,0} → 2p1 3s1 ¹ P _{1,0}	pec96#c_vsr#c2.dat
4326.8Å	C ²⁺	2p1 3p1 ¹ D _{2,0} → 2p1 3s1 ¹ P _{1,0}	pec96#c_vsu#c2.dat

OPEN-ADAS

Atomic Data and Analysis Structure

OPEN-ADAS Version 1.0

[Report Error](#) | [My Account](#) | [Log Out](#)

Freeform search

Search by wavelength

Search by ion

Search by data class

Documentation

Download code

Terminology

Statistics

About ADAS

About OPEN-ADAS

ADF01	ADF04	ADF07	ADF08	ADF09	ADF11	ADF12	ADF13	ADF15	ADF21	ADF22
-------	-------	-------	-------	-------	-------	-------	-------	--------------	-------	-------

ADF15 File: pec96#c_vsr#c2.dat

Photon Emissivity Coefficients

Ion: C²⁺
 Temperature Range: 0.388 eV → 2330 eV
 Density Range 2.19 x 10⁴ cm⁻³ → 2.19 x 10¹⁸ cm⁻³
 Filename: pec96#c_vsr#c2.dat
 Full Path: adf15/pec96#c/pec96#c_vsr#c2.dat

Download Options

[Download Data](#)
[Documentation](#)
[Software libraries](#)

[Show comments](#) | [Show origins](#)

Wavelength	Transition	Type	Driving Population
2010.5Å	2s1 4s1 ³ S _{1,0} → 2s1 3p1 ³ P _{4,0}	Excitation	2s2 ¹ S _{0,0}
2010.5Å	2s1 4s1 ³ S _{1,0} → 2s1 3p1 ³ P _{4,0}	Excitation	2s1 2p1 ³ P _{4,0}
2010.5Å	2s1 4s1 ³ S _{1,0} → 2s1 3p1 ³ P _{4,0}	Recombination	
2010.5Å	2s1 4s1 ³ S _{1,0} → 2s1 3p1 ³ P _{4,0}	Charge Exchange	
2092.7Å	2s1 4p1 ³ P _{4,0} → 2s1 3d1 ³ D _{7,0}	Excitation	2s2 ¹ S _{0,0}
2092.7Å	2s1 4p1 ³ P _{4,0} → 2s1 3d1 ³ D _{7,0}	Excitation	2s1 2p1 ³ P _{4,0}
2092.7Å	2s1 4p1 ³ P _{4,0} → 2s1 3d1 ³ D _{7,0}	Recombination	

OPEN-ADAS

Atomic Data and Analysis Structure

OPEN-ADAS Version 1.0

[Report Error](#) | [My Account](#) | [Log Out](#)

Freeform search

Search by wavelength

Search by ion

Search by data class

Documentation

Download code

Terminology

Statistics

About ADAS

About OPEN-ADAS

Wavelength

Minimum (Å) → Maximum (Å)

Resolve Results By

Transition (longer list)

File (shorter list)

Wavelength	Ion	Data Type	Transition	File Details
4946.1Å	Ne ¹⁰⁺	ADF12	14 → 12	qef97#h_en2_kvi#ne10.dat
4973.1Å	Li ⁰⁺	ADF13	1s2 4s1 ² S _{0.5} → 1s2 2p1 ² P _{2.5}	sxb96#li_pjr#li0.dat
4973.1Å	Li ⁰⁺	ADF15	1s2 4s1 ² S _{0.5} → 1s2 2p1 ² P _{2.5}	pec96#li_pju#li0.dat
4973.1Å	Li ⁰⁺	ADF13	1s2 4s1 ² S _{0.5} → 1s2 2p1 ² P _{2.5}	sxb96#li_pju#li0.dat
4973.1Å	Li ⁰⁺	ADF15	1s2 4s1 ² S _{0.5} → 1s2 2p1 ² P _{2.5}	pec96#li_pjr#li0.dat
5010Å	He ⁰⁺	ADF22	1s3p ¹ P → 1s2s ¹ S	nm501_m1s#he_o8.dat
5010Å	He ⁰⁺	ADF22	1s3p ¹ P → 1s2s ¹ S	nm501_m2f#he_c6.dat
5010Å	He ⁰⁺	ADF22	1s3p ¹ P → 1s2s ¹ S	nm501_m3s#he_h1.dat
5010Å	He ⁰⁺	ADF22	1s3p ¹ P → 1s2s ¹ S	nm501_m1f#he_o8.dat
5010Å	He ⁰⁺	ADF22	1s3p ¹ P → 1s2s ¹ S	nm501_m1s#he_h1.dat

Freeform search

Search by wavelength

Search by ion

Search by data class

Documentation

Download code

Terminology

Statistics

About ADAS

About OPEN-ADAS

OPEN-ADAS Freeform Search

neutral be influx visible

Search

Total results found: 469
Recommended results: 14
Other results: 455

Recommended files

Ion	Reasons	Type of data	File
Be ⁰	Ion: Be ⁰ S/XB transition at: 4573.9Å Influx measurement data S/XB transition at: 6475.2Å S/XB transition at: 4409.2Å S/XB transition at: 6475.2Å	Ionisation Per Photon Coefficients	sxb96#be_pjr#be0.dat
Be ⁰	Ion: Be ⁰ S/XB transition at: 4573.9Å Influx measurement data S/XB transition at: 4409.2Å S/XB transition at: 6475.2Å	Ionisation Per Photon Coefficients	sxb96#be_pju#be0.dat
Be ⁰	Ion: Be ⁰ S/XB transition at: 4573.9Å Influx measurement data S/XB transition at: 4409.2Å S/XB transition at: 4573.9Å	Ionisation Per Photon Coefficients	sxb93#be_llr#be0.dat
Be ⁰	Ion: Be ⁰ S/XB transition at: 4409.2Å S/XB transition at: 4573.9Å Influx measurement data	Ionisation Per Photon Coefficients	sxb93#be_pjr#be0.dat
Be ⁰	Ion: Be ⁰ S/XB transition at: 4409.2Å Influx measurement data	Ionisation Per Photon Coefficients	sxb93#be_llu#be0.dat

Beta testing

- Had a very successful beta testing process over the summer.
- The beta-test proved incredibly worthwhile with excellent feedback from all people concerned — thank you again.
- Some ‘representative’ comments:
 - **“First off, kudos for a phenomenal job. The interface is easy to use and clear, and the pages are nicely clean.”**
 - **“Overall, the site is very clean and efficient. Very well done.”**
- Some were slightly more technical, we think every point was acted on and answered satisfactorily.

Usage as of 25th September 2008

- So far we have 26 registered users (including 12 from the betatesting process):

Austria	2	China	2	France	1	Germany	4
Japan	1	Portugal	1	Scotland	2	Switzerland	2
UK	3	US	1	USA	7		

- Not bad considered no advertising done so far, the only thing we did was add a link from the main ADAS webpage.
- Web server running 24/7 since launch with no problems.
- For the month of August:
 - 10,471 individual requests: average of 14 requests per hour,
 - However: 8,633 of these requests were Google indexing everything.

'Data integrity'

- Slight change of topic but very much related to OPEN-ADAS.
- Main topic is data but code integrity is also an issue.
- Some things I'd like to cover are:
 - Documentation
 - ADAS members copying data out of ADAS and then not updating it,
 - Allowing access to our CVS repositories,
 - Correcting errors in data downloaded from OPEN-ADAS.

—
Summers → Lauro-Taroni → Strachan → Coster → Bonnin
would be better as
Summers ↔ ADAS ↔ Bonin

Documentation

Currently ADAS data contains comments like:

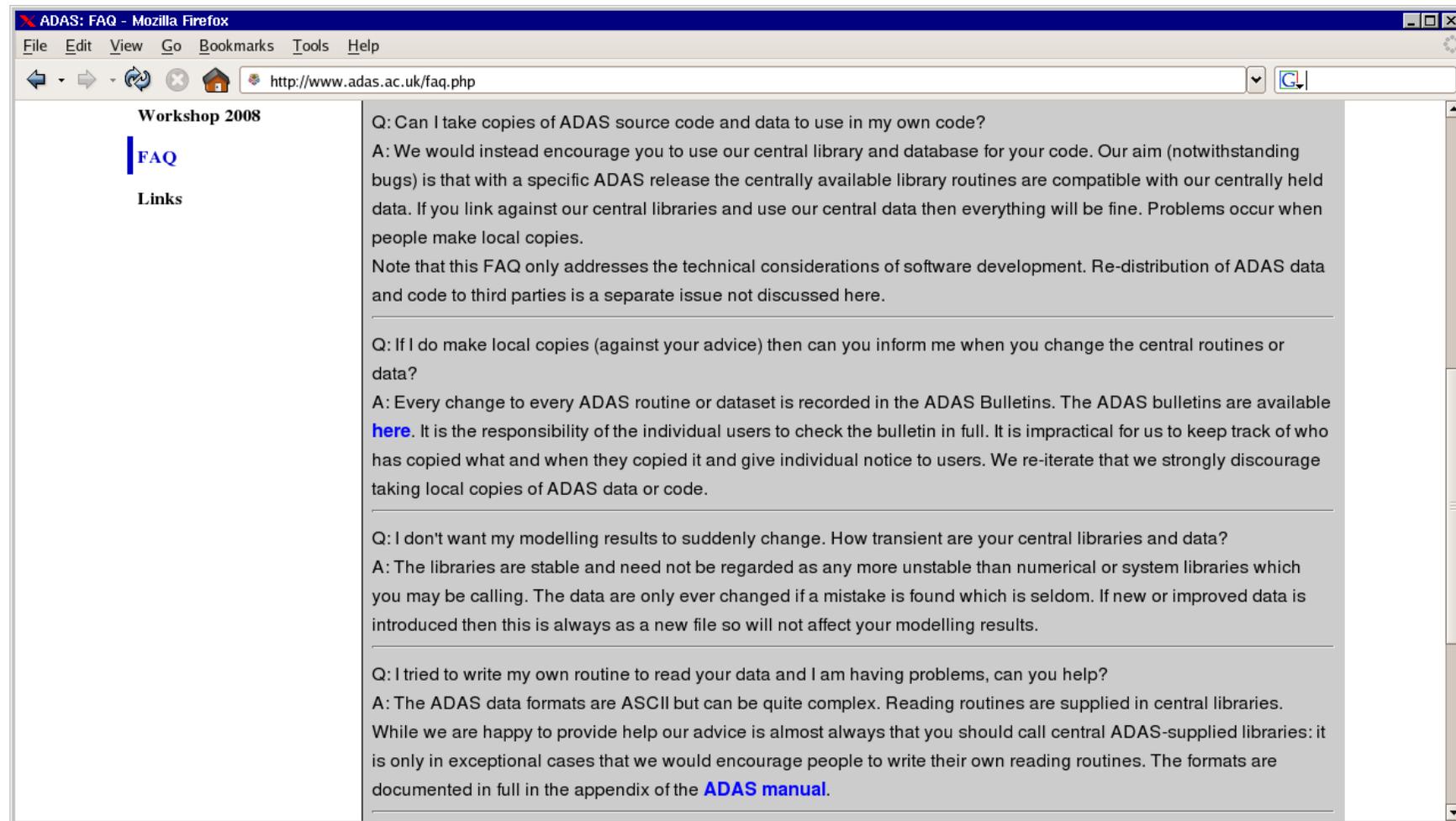
```
C      N. R. BADNELL, D. C. GRIFFIN & D. M. MITNIK J.PHYS.B36 1337-50 (2003).
```

which gives a reference a human can follow but not a machine. We want to add DOI numbers to every file:

```
C      M C Witthoeft, A D Whiteford and N R Badnell  
C      J Phys B 40 2969-2993 (2007)  
C      DOI: 10.1088/0953-4075/40/15/001
```

- We can automatically parse a DOI to get title, authors etc.
- Will appear as clickable links in OPEN-ADAS and perhaps some kind of official ADAS bibliography.

Copying data...



However, let's build bridges rather than walls...

- We do realise there are often compelling reasons to take local copies of our data/codes, e.g.:
 - Using our pre-compiled libraries is impractical on large computer systems with strange compiler options,
 - ADAS is sometimes installed on a remote PC which is inconvenient when trying to do local analysis,
 - The data need to be used in a larger organised framework which requires a local copy (e.g. ITM).
- Suggesting that you need to make your own archived copies of ADAS data/code in case it changes is less sensible: you are not going to backup your system libraries, numerical libraries, compiler toolchain etc. etc. so why single ADAS out as some kind of weak-link?

Controlled release of data and code

- ADAS Project members:
 - We want to give access to our CVS repositories
 - Not quite as simplistic as just going login details — we have created CVS views which expose related cross-sections of our archive in a (we think) user friendly way.

- OPEN-ADAS:
 - We record exactly who has downloaded what file and when.
 - Terms and conditions of OPEN-ADAS restrict redistribution to maximise data integrity.
 - The plan is that if we find an error we can e-mail everyone who has downloaded that file.
 - Recommendation to allow anonymous access with sufficient health warnings.

CVS views

The routines to read an ADF04 file are:

```
fortran/adaslib/xxdata/xxdata_04.for   fortran/adaslib/utility/xxpars.for   fortran/adaslib/system/i4unit.for
fortran/adaslib/utility/xxword.for     fortran/adaslib/utility/xxslen.for   fortran/adaslib/atomic/xxprs1.for
fortran/adaslib/utility/r8fctn.for     fortran/adaslib/utility/i4fctn.for   fortran/adaslib/atomic/i4idfl.for
fortran/adaslib/utility/xxpars.for     fortran/adaslib/utility/xxrmve.for   fortran/adaslib/utility/xxcase.for
```

it's clearly non-practical to have people know or navigate this.

Instead we create a 'CVS view' which puts all of the above into a flat module which one would get via:

```
cvs -d username@cvs.adas.ac.uk co /views/xxdata_04
```

full revision histories etc. are still available, from the point of view of the user they may as well have access to a conventional CVS repository.

Note: we made up the terminology 'CVS views' but we quite like it.

Conclusions and discussion points

- OPEN-ADAS v1.0 is released and the final report complete.
- There will, of course be version 1.1 incorporating many of the suggestions which didn't make it into version 1.0.
- We hope direct CVS access will improve matters. But, we do emphasize that we supply pre-compiled libraries and extensive (~ 1500 pages) documentation for these libraries.
- Anonymous access to OPEN-ADAS — are some people too lazy to register?
 - Probably — but do we even care about people who are such casual users?

Thank you!