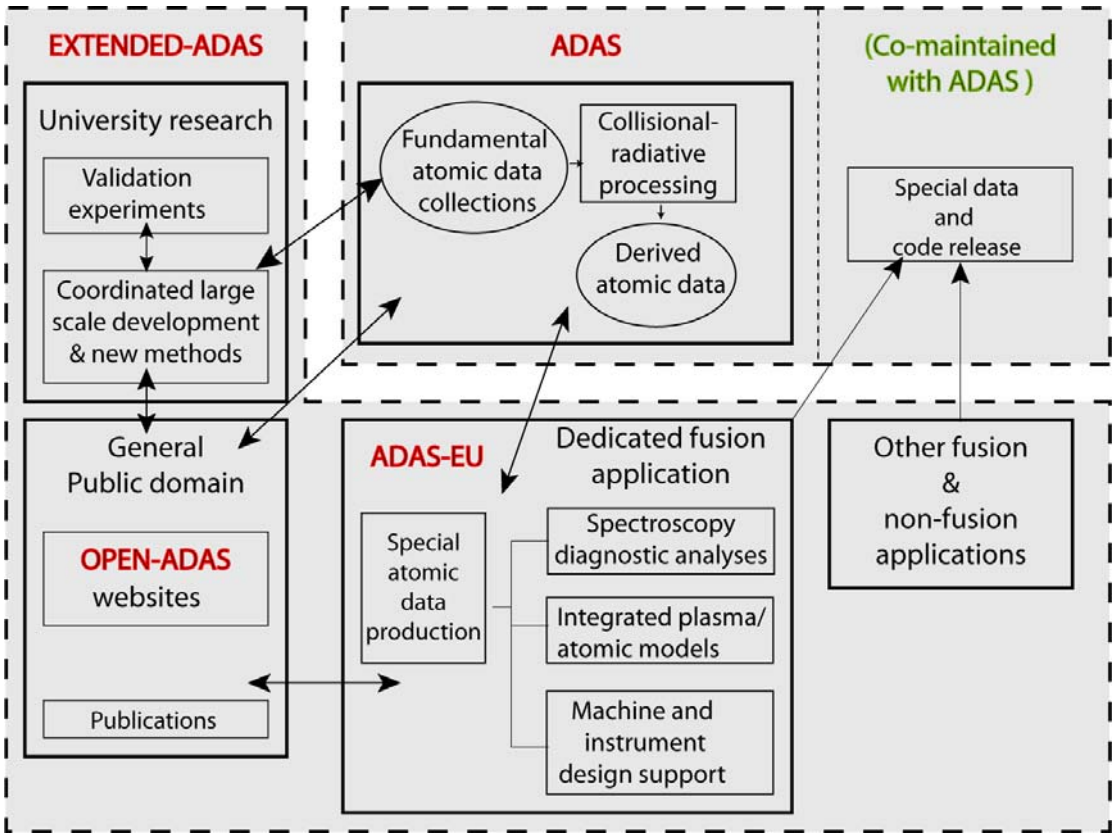
Dec12-08 **ADAS Bulletin**

In this bulletin, as well as detailing ADAS code additions and corrections and extensions to the ADAS database, I wish to present what has been happening under the headings OPEN-ADAS, EXTENDED-ADAS and ADAS-EU. For those of you who have not been at the last two ADAS Workshops and exposed to my overview talks, some clarification may be required.

The chart below shows the relationships. ADAS is the core part of fundamental and derived atomic data with the ADAS codes which take one from the former to the latter. The derived data are the various coefficients required by plasma models or by diagnostic spectroscopy. They are collisional-radiative quantities which depend only on local plasma conditions of electron temperature, electron density and so on. Such a boundary makes good sense, since it separates what is of general value and applicability from what is specific to a particular machine or diagnostic device. But of course to procure the fundamental data needed for ADAS and to ensure that the atomic data ADAS provides is tested and checked, the ADAS Project has had to look beyond the boundary. I call this EXTENDED-ADAS. On the schematic it surrounds ADAS and has links back and forth to it. The University research part of EXTENDED-ADAS, we are all familiar with. For many years, the ADAS Project has been assiduous in establishing and promoting these key activities. Indeed with our academic hats on, with many research students and colleagues around the world, we have developed and implemented some very effective coordinated production. Also, you will have been aware of some of the application codes, such as SANCO (the 1-D impurity transport code), UTC (the universal transport analysis code) and now CXSFIT (the charge exchange spectral fitting code). CXSFIT, signalled as pretty well operational a year ago, with a first cut at its manual, has been extensively worked with at JET, IPP Garching and Juelich over the past year. It is now robust and with a full detailed manual out at IPP (IPP.10-36 July 2008) and currently on its way out as an EFDA-JET report. In the appendix at the end, I have copied just the front and contents pages.



CXSFIT is in the character of a fusion application, which is co-maintained with ADAS. It requires certain tokamak device specific experimental data acquisition procedures to connect with its universal

core fitting. This requires some specific collaboration between experimentalists wishing to use such codes and ADAS staff. Martin O'Mullane maintains SANCO. Allan Whiteford maintains UTC and CXSFIT. They are not part of ADAS itself, but ADAS Project members in other laboratories are welcome to use them and are strongly invited to talk with central ADAS about getting them and finding out how to use them. Right now, it is CXSFIT which is the new code in town (developed by Allan with lots of input from Manfred, Klaus-Dieter and Lorne) of which we are rather proud.

The past year has seen us put large efforts into OPEN-ADAS and preparing ADAS-EU, which are again parts of EXTENDED-ADAS. I am pleased to note in this bulletin that OPEN-ADAS is now released. Also we have a substantial manual accompanying the release from which I have again clipped the cover and contents pages for the appendix of this bulletin. We are very obliged to those of you who beta-tested it. OPEN-ADAS is a shared development with ADAS and IAEA created by Allan Whiteford. It makes available in the public domain relevant parts of the ADAS derived database. OPEN-ADAS also fulfils the wish for easier location of the appropriate data (out of the now very large ADAS database) by the ADAS user. Note the web address http://open.adas.ac.uk. Incidentally, ADAS now has its own top level academic web addresss http://www.adas.ac.uk.

So we come to ADAS-EU, which represents EURATOM and the European Commission getting interested in ADAS and viewing it as a route to providing the necessary atomic physics support to fusion across Europe and as a European contribution to ITER. I have been working for a year on designing a plan for ADAS for Fusion in Europe (ADAS-EU) and negotiating contract details. I am pleased to say that the contract was signed on 5 Dec. and ADAS-EU will commence on 1 Jan. 2009. In the chart above you will see how ADAS-EU fits in. It is part of EXTENDED-ADAS, supporting and developing the effective application of ADAS in fusion research establishments in Europe and at ITER. It is, and must be, independent of ADAS itself, and the direct support must be to European Associated Laboratories of EURATOM, but the product of ADAS-EU will be made available to all ADAS members, through ADAS itself and relevant data generated by it will appear in the public domain through OPEN-ADAS.

Figure 1 ADAS-EU: Physics theme and sub-theme support time chart

Theme	Code	Actions	2009	2010	2011	2012
Heavy element [1] spectroscopy and models	T1	applic.		Superstages & emissivities		Global scaling
		fund.	Baseline & emissivities[2]	Ionisation level 1	DR/GBPP level 1	Neutrals, level 2
		exploit.[3]	Heavy species in ITER studies	Tungsten spectral emission (ASDEX-U, JET)	Atomic model support of ITM for ITER	
Charge exchange spectroscopy	T2	applic.	CXSFIT shared analysis Parametric CXS	NEW-CHEAP shared analysis	CXS/UTC/transport link	
		fund.	Bundle-n & l-mix models	CTMC (improved) /CCAO/CCMC	Bundle-nl models for partially stripped receivers	
		exploit	CXS line fittiing extended to argon	Multi-line CXS region observation	Cross-linked CXS & passive diagnostic	
Beam stopping beam emission spectroscopy	T3	applic.		Li/Na beam analysis and database	Beam emission/beam stopping consistency	
		fund.	Li/Na beam database	Bundle-n & Stark GCR		
		exploit.		Li/Na beam edge parameter diagnosis	Beam emission exploitation for ITER	
Special features	T4	applic.			Integrated special feature fitting and display	
		fund.		Zeeman, soft-X-ray, Balmer series special features		
		exploit.	Fitting with spectral primitives	He-like soft X-ray line analysis	Balmer series/limit observations	
Diatomic spectra and coll-rad models	T5	applic.		H_2 isotopomer spectral simul.		
		fund.	H_2/H electr. & ion database	H_2/H vibronic/GCR populations		
		exploit.		Composite continuum emission studies	Integrated edge modelling	

Notes: (1) Sets of 3 to 5 work packages make up the scientific support of each theme. Each work package is sub-divided into tasks.
(2) The completion of the sub-themes in the 'applic.' and 'fund.' categories mark science milestones. The sub-theme is an assembly of work package tasks.
(3) 'exploit' indicates the expected use by fusion plasma modellers and spectral diagnosticians on-site at European fusion laboratories, with which ADAS-EU staff will assist.

The ADAS-EU Support Action will last for four years and will be provided by the University of Strathclyde. It will enable us to put about 12 man-years of extra-effort into atomic physics support for fusion as well as enabling some modest special data commissioning from specialist University departments. Martin, Allan and I will assign part of our time to be being (working) project managers. Professor Ratko Janev will be a part-time visiting professor of Strathclyde University, helping with molecular and ion impact data parts of ADAS-EU. ADAS-EU will employ two new post-doctoral researchers who will be physically based at European laboratories – one divided between Juelich/Cadarache/ITER and the other at IPP Garching. They will play a role like Martin O'Mullane does for JET. **So we will be recruiting in the early New Year. Please draw this to the attention of any prospective candidates you know of are have in your laboratories or groups. I shall circulate**

a job specification and invitation to apply soon. ADAS-EU will allow us to provide much closer support, with frequent on-site visits to other European fusion laboratories. We will be able to sustain regular annual ADAS and atomic modelling training courses with more staff to which all ADAS members will be welcome to send participants. Also there will be no reduction of our interaction with ADAS members outside Europe, to which the other part of Allan, Martin and my time is committed.

To complete the ADAS-EU story, I show in the figure above, the main themes which will be followed in the four years of ADAS-EU and executed in a number of work packages and deliverables. There is of course much more detail which can be discussed in future occasions. Lastly, to make this a success, we shall of course need to employ strong postdoctoral researchers who will be prepared and at their peaks by the time ITER comes along. I shall be advertising these posts very early in the New Year and encourage you all to get your good postdocs to apply.

Returning to core ADAS, the present release has a lot of small additions and corrections and a significant amount of new data. I draw particular attention to the argon CXS data - some of it comparative. We do not have enough clarity yet on CXS for heavier species, but the data given here is the best we can do (and our preferred data for testing) against the experimental studies in the pipeline at AUG and JET. I trust it will be useful. The code tidying up is partly for the benefit of OPEN-ADAS (downloads and so on), but also a prelude to our next release – due in March 2009. The March release will be one of the largest releases we have had (since the original JET-ADAS conversion) with many new codes. It will provide a complete capability for heavy species modelling and substantial heavy species data. Adam Foster and I are working on the adjustments, links and checks for embedding all the new codes into central ADAS now. It will be called release 3.0, since it rationalizes and unifies quite a bit of previous ADAS practice particularly at the IDL command line level. Those of you who would like a preview of some of its content might like to look at Adam's PhD Thesis which is available now on the ADAS web-site,

The list of code and data updates follows:

1. Code and data updates in v2.13.

Corrections and updates to code (ADAS v2.12 to ADAS v2.13)

C.1 *run_adas406.pro* failed when extracting the partition information when implicit file naming (user, year, element etc.) was used but worked if the files structure was input.

C.2 Added *c4spln.for* to adas3xx compiled libraries.

C.3 Increased length of *strg* to 1024 in *fortran/adaslib/atomic/xxrptn.for*

C.4 Added include directory and put in some basic C prototypes for Fortran subroutines:
adaslib.h:*continuo, xxdata_21* and *xxopen*
adas3xx.h:*cxbms*

C.5 Added C++ top level directory and adas3xx sub-directory. The C++ directory will mirror the current C directory.

C.6 Added *C++/adas3xx/cxbms.cpp* and i*nclude/cxbms.hpp* which are C++ class wrappers to the *cxbms* subroutine.

C.7 Added a 'makecpp' script in the make_release directory which compiles all (currently only one) C++ routines into a library in 'lib/libadascpp.a'.

C.8 Added *makecpp* to *makeall*.

C.9 Modified subroutine library documentation to include more extensive information on calling ADAS routines from Fortran, C and C++. Included more C examples (reading and ADF21 file and calculating beam stopping) and one C++ example using the *cxbms.cpp* class wrapper.

C.10 Allowed subroutine library documentation to generate a separate document which is only the linking information.

C.11 Modified ADAS303 to use updated version of *xxdata_12*.

C.12 Add a run_adas414.pro and write_adf35.pro to enable the generation of power filter functions in a scriptable way.

C.13 Added *adas603_get_multiplets* to programatically return a list of features ADAS603 can calculate.

C.14 Moved splitting of routines in *makelib* compilation script for better compatibility with Sun implementation of csh.

C.15 Changed loop variable from int to long to allow for more than 32,768 levels in:
idl/adas2xx/adas206/cw_adas206_proc.pro
idl/adas2xx/adas206/b6ispf.pro

C.16 Changed loop variable from int to long to allow for more than 32,768 rows in:
idl/adaslib/text_table.pro

C.17 Added purpose to the comments for routines:
fortran/adas1xx/adas102/esolve1.for
fortran/adas1xx/adas102/esolve2.for
and removed 0s from columns 72-80.

C.18 Minor changes to comments of:
wrapper/read_adf/read_adf24/readadf24.for

C.19 Made a new *xxdata_07.for* routine which is more or less a direct copy of *e2data.for* and has an identical API.

C.20 Removed *e2data.for* and entry in *makelib*.
WARNING: *e2data* is no longer in the adas5xx library, use *xxdata_07* from adaslib library instead.

C.21 Changed codes which did use *e2data* to now use *xxdata_07*, specific changes were made to:
fortran/adas2xx/adas204/b4sszd.for
fortran/adas2xx/adas204/comp204
fortran/adas2xx/adas208/adas502v208.for
fortran/adas2xx/adas208/comp208
fortran/adas3xx/adas310/casszd.for
fortran/adas3xx/adas310/comp310
fortran/adas3xx/adas311/comp311
fortran/adas5xx/adas502/adas502.for
fortran/adas5xx/adas502/comp502
fortran/adas5xx/adas502/e2setp.for
fortran/adas5xx/adas502/sszd.for
wrapper/read_adf/read_adf07/comp_read_adf07
wrapper/read_adf/read_adf07/readadf07.for

C.22 Add *fulldata* output structure to *read_adf07.pro*. An accompanying *xxdata_07.pro* is also available.

C.23 Removed *fortran/adas5xx/adas502/sszd.for* from list of routines compiled into adas502v208 from comp208 script.

C.24 Small modification to comments of:
fortran/adas8xx/adas804/fcf4.for

C.25 Made a new *xxdata_08.for* routine which is more or less a direct copy of *dbdata.for* and has an identical API.

C.26 Removed *dbdata.for* and entry in makelib.
WARNING: *dbdata* is no longer in the adas4xx library, use *xxdata_08* from adaslib library instead.

C.27 Changed codes which did use *dbdata* to now use *xxdata_08*, specific changes were made to:
fortran/adas4xx/adas411/adas411.for
fortran/adas4xx/adas411/comp411
wrapper/read_adf/read_adf08/readadf08.for
wrapper/read_adf/read_adf08/comp_read_adf08

C.28 Modification to *xxdata_01* so that it can correctly parse files which contain m-subshell data and print a warning saying that the m-resolved data were ignored.

C.29 Introduce an *xxdata_19*.for routine which is more or less a direct copy of *e4data.for* and has an identical API. IDL versions, along with a read_adf19.pro and *write_adf19.pro* are also included.

C.30 Changes to *xxdata_15*, to allow handling of partitioned data, caused unexpected changes to adas409 code to generate GTN data.

C.31 The fortran utility routine, *i4indfi4.for*, which finds the index in an integer array corresponding to the exact match of a requested value no longer assumes that the input array is monotonic.

C.32 Added /cache keyword to *read_adf0.pro*

C.33 Added *cfg2occ* routine.

C.34 Added *ignore_untied* keyword to IDL *read_adf04.pro* routine

C.35 Allowed IDL *xxdata_04.pro* routine to handle adf04 files which contain zero transitions.

C.36 Modified Fortran *xxdata_04.for* routine to allow ionisation potential to be zero for bare nuclei and also allowed for configuration strings being empty (also required for ADAS bare nuclei files).

C.37 User supplied temperatures to adas801 (Cowan code) occasionally resulted in an error if fewer than (the maximum of) 14 were set.

C.38 Fixed bug in maximum allowed occupation in *adas8#3* script. Added example output to *adas8#3* script

C.39 Update the data reading/interpolation branch of *read_adf11.pro* to use the latest version of *xxdata_11.for*. All resolved, standard and bundled datasets can now be read. Note that the new nomenclature for partition data is enabled but the old names will also work. A */nocheck* option is provided for the brave.

C.40 Added *adas_string_justify.pro* to split a scalar string into a string array with each element having a maximum number of characters and the splitting done on word breaks.

C.41 Added *cw_adas_multilabel.pro* for producing multi line text widgets.

C.42 Error in an internal diemension in *xxdata_15.pro* which could result in corrupted density values in the *fulldata* structure.

C.43 Corrected logic in *occ2cow.pro* for rare gas omitted-shell detection Further correction to logic for Cowan effective z for driver. Now use zc=z1 for z0<19.

C.44 Added --root option to *adas8#3* and made --archive option more sensible.

C.45 Increase the number of transitions in input adf04 datasets to 3000. Correct an un-initialised variable fault which caused problems on some platforms.

C.46 Add an IDL version of *r8fbch.for*, which evaluates the shell contribution to the ionisation rate coefficient in the Burgess-Chidichimo approximation. Similar to *r8necip.pro* the IDL version allows a vector of temperatures while the fortran routine is limited to a single temperature.

C.47 Added *auto_wave* keyword to automatically generate a wavelength grid (i.e. no need for wave_min and wave_max) and added *wave_doppler* keyword to return the wavelength grid (works for either an automatically generated grid or a manually supplied wave_min/ wave_max) to *adas305_get_stark.pro* IDL routine.

C.48 Error when printing the graph to a file in adas304 is fixed.

C.49 Add *config_orbital_energies.pro*, a routine to calculate the orbital energies for a given configuration. Note that it uses one step of the Cowan code (adas801) for this.

C.50 An IDL routine to write adf12 datasets, with input data in form of adf12 fulldata structure, has been added: *write_adf12.pro*. A helper routine, *trim_adf12.pro*, has been provided to limit the adf12 output from adas316 to more a manageable size. The top n lines, or a list of n-n' transitions can be used.

C.51 Add a *run_adas312.pro* to enable the the post-processing of adf26 datasets to produce beam stopping (adf21) and beam emission and excited populations (adf22) coefficients via an IDL script.

C.52 *read_adf01.pro* would fail if more than 100 energies were requested. It now reads data in chunks, like the other read_adf routines, to avoid this problem.

C.53 Increased version number to 2.13.

Corrections and updates to data (ADAS v2.12 to ADAS v2.13)

D.1 Renamed *adf01/qcx#h0/qcx#h_ar18.dat* to *qcx#h0_and#ar18.dat*

D.2 Changed labelling of "keV.amu" to "keV/amu" in:
adf01/qcx#he0/qcx#he0_kvi#he2.dat
adf01/qcx#na0/qcx#na0_kvi#he2.dat

D.3 Changed erroneous "nmin" label to "nmax" in:
adf01/qcx#he0/qcx#he0_2s-s_kvi#c6.dat

adf01/qcx#he0/qcx#he0_2s-s_kvi#he2.dat
adf01/qcx#he0/qcx#he0_2s-t_kvi#c6.dat
adf01/qcx#he0/qcx#he0_2s-t_kvi#he2.dat
and also removed DOS carriage returns

D.4 Fixed ISEL indexing in comments of:
adf07/szd93#c/szd93#c_c1.dat

D.5 Removed "CC" from some of the comment lines of:
adf07/ionelec/ionelec_szd#o.dat

D.6 Added F-like sequence adf04 data:
adf04/copaw#f/flike_mcw06#al4.dat
adf04/copaw#f/flike_mcw06#ar9.dat
adf04/copaw#f/flike_mcw06#as24.dat
adf04/copaw#f/flike_mcw06#br26.dat
adf04/copaw#f/flike_mcw06#ca11.dat
adf04/copaw#f/flike_mcw06#cl8.dat
adf04/copaw#f/flike_mcw06#co18.dat
adf04/copaw#f/flike_mcw06#cr15.dat
adf04/copaw#f/flike_mcw06#cu20.dat
adf04/copaw#f/flike_mcw06#fe17.dat
adf04/copaw#f/flike_mcw06#ga22.dat
adf04/copaw#f/flike_mcw06#ge23.dat
adf04/copaw#f/flike_mcw06#k10.dat
adf04/copaw#f/flike_mcw06#kr27.dat
adf04/copaw#f/flike_mcw06#mg3.dat
adf04/copaw#f/flike_mcw06#mn16.dat
adf04/copaw#f/flike_mcw06#na2.dat
adf04/copaw#f/flike_mcw06#ne1.dat
adf04/copaw#f/flike_mcw06#ni19.dat
adf04/copaw#f/flike_mcw06#p6.dat
adf04/copaw#f/flike_mcw06#s7.dat
adf04/copaw#f/flike_mcw06#sc12.dat
adf04/copaw#f/flike_mcw06#se25.dat
adf04/copaw#f/flike_mcw06#si5.dat
adf04/copaw#f/flike_mcw06#ti13.dat
adf04/copaw#f/flike_mcw06#v14.dat
adf04/copaw#f/flike_mcw06#zn21.dat

D.7 Added Ca-like Fe file:
adf04/calike/calike_mcw07#fe6.dat

D.8 Added Mg-like DR sequence adf09 datasets:
adf09/za00#mg/za00#mg_<ion> <resol><nn'n''>.dat
where <*ion*> is *al1, ar6, ca8, cl5, co15, cr12,cu17, fe14, k7, kr24, mn13, mo30, ni16, p3, s4, sc9, si2, ti10, v11, xe42, zn18*
and <*resol*> is *ls, ic*
and <*nn'n''*> is *23, 334*

along with adf27 drivers for ADAS701 :
adf27/dr/mglike/za00#mg/<ion> <resol><nn'-n''>e.dat
adf27/dr/mglike/za00#mg/<ion> <resol><nn'-n''>o.dat
adf27/dr/mglike/za00#mg/<ion> <resol><nn'-n''>str.dat
where <*ion*> is *al1, ar6, ca8, cl5, co15, cr12,cu17, fe14, k7, kr24, mn13, mo30, ni16, p3, s4, sc9, si2, ti10, v11, xe42, zn18*
and <*resol*> is *ls, ic*
and <*nn'-n''*> is *23-3, 23-n, 34-34, 34-n*

and adf28 drivers for ADAS702:

adf28/dr/mglike/za00#mg/<ion> <resol><nn'-n''>e.dat
adf28/dr/mglike/za00#mg/<ion> <resol><nn'-n''>o.dat
adf28/dr/mglike/za00#mg/<ion> <resol><nn'-n''>str.dat

where <*ion*> is *al1, ar6, ca8, cl5, co15, cr12,cu17, fe14, k7, kr24, mn13, mo30, ni16, p3, s4, sc9, si2, ti10, v11, xe42, zn18*
and <*resol*> is *ls, ic (or icm)*
and <*nn'n''*> is *23, 334.*

As always, significant re-naming of the files were done from the originals.

D.9 Added Mg-like RR sequence adf48 datasets:

adf09/nrb05#mg/nrb05#mg_<ion> <resol>.dat

where <*ion*> is *al1, ar6, ca8, cl5, co15, cr12,cu17, fe14, k7, kr24, mn13, mo30, ni16, p3, s4, sc9, si2, ti10, v11, xe42, zn18*
and <*resol*> is *ls, ic*

along with adf27 drivers for ADAS701 :

adf27/rr/mglike/nrb05#mg/<ion> <resol>-3.dat
adf27/rr/mglike/nrb05#mg/<ion> <resol>-n.dat
adf27/dr/mglike/nrb05#mg/<ion> <resol>_str.dat

where <*ion*> is *al1, ar6, ca8, cl5, co15, cr12,cu17, fe14, k7, kr24, mn13, mo30, ni16, p3, s4, sc9, si2, ti10, v11, xe42, zn18*
and <*resol*> is *ic*

and adf28 drivers for ADAS702:

adf28/rr/mglike/za00#mg/<ion> <resol>.dat

where <*ion*> is *al1, ar6, ca8, cl5, co15, cr12,cu17, fe14, k7, kr24, mn13, mo30, ni16, p3, s4, sc9, si2, ti10, v11, xe42, zn18*
and <*resol*> is *ls, ic*

D.10 The ionisation potentials in the adf00 datasets for medium to high Z ions are generally taken from a 1970's compilation. For many elements this is still the only reference but better data exists for some favoured elements. Xenon data now comes from E Saloman, J. Phys. Chem. Ref. Data,', Vol. 33, No. 3, 2004.

D.11 Minor changes to the adf39 entry in Appendix A to correct the definition of some of the parameters.

D.12 Brought list of transitions in the comments into line with the more standard layout of including the configuration and term in the Fe adf07 files:

adf07/szd93#fe/szd93#fe_fe.dat
adf07/ionelec/ionelec_szd#fe.dat

D.13 Update to:

adf04/calike/calike_mcw07#fe6.dat

Fixed radiative transitions involving levels 25 and 26 which were erroneously swapped in the radiative rate calculation.

D.14 One of the temperatures in *adf19/ionelec/ionelec_pzd#c.dat* was out of sequence. This temperature point has been removed from the dataset. The existing dataset was changed as this was considered to be an error.

D.15 The file:

adf04/mglike/mglike_al97#fe14.dat

actually contained data for (Na-like) Fe15+. The file has been modified internally to reflect this and moved to:

adf04/nalike/nalike_al97#fe15.dat

D.16 Moved comments to first column, added note about data quality and removed parentage information from level list from:

belike/belike_mom92b.dat
belike/belike_mom92be.dat
blike/blike_mom92b.dat
clike/clike_mom92c.dat
olike/olike_mom92o.dat

D.17 Fixed configuration specification (n=3 levels were incorrectly labelled like n=2 levels) in *adf04/helike/helike_adw00#s14.dat*

D.18 Removed extra whitespace from some of the data in *adf04/helike/helike_adw02#o6.dat*

D.19 Changed level specification from simple '1', '2' etc. to 'n=1', 'n=2' etc. in:

adf04/hlike/hlike_bn#l91h.dat
adf04/hlike/hlike_bn#h91h.dat

D.20 Removed periods from configuration specifications in:

adf04/mglike/mglike_al97#ar6.dat

D.21 Tidied up level listing by removing '-' sign from configurations, fixing whitespace issues and removing parentage information in:

adf04/blike/blike_wjd92#o.dat

D.22 Fixed formatting on first line of *adf04/blike/blike_jl1989o.dat*

D.23 Added Ne-like adf04 dataset, a Dirac-Fock R-Matrix calculation of Connor Ballance and Don Griffin for Fe. It is archived in *adf04/nelike/nelike_cpb06#fe16.dat*

Added adf15, in the low level metastable unresolved picture, for this dataset (in the 15-18A) range to *adf15/transport/transport_llu#fe16ic.dat*

D.24 Updated files:

adf09/za00#mg/za00#mg_ar6ic23.dat
adf09/za00#mg/za00#mg_ar6ls23.dat *
adf09/za00#mg/za00#mg_cl5ic23.dat
adf09/za00#mg/za00#mg_cl5ls23.dat
adf09/za00#mg/za00#mg_xe42ic23.dat *
adf09/za00#mg/za00#mg_xe42ls23.dat

to deal with problem of NULL characters appearing. Note that the above files marked with a * did not suffer this problem but were re-calculated anyway with a newer version of *adasdr* which gives slightly different structure. They were hence also updated to maintain consistency.

D.25 Updated files:

adf28/dr/mglike/za00#mg/ar6icm23.dat
adf28/dr/mglike/za00#mg/ar6ls23.dat
adf28/dr/mglike/za00#mg/cl5icm23.dat
adf28/dr/mglike/za00#mg/cl5ls23.dat
adf28/dr/mglike/za00#mg/xe42icm23.dat
adf28/dr/mglike/za00#mg/xe42ls23.dat

to deal with problem of *adasdr* potentially finding too many targets (now fixed in latest version of *adasdr*).

D.26 Add adf15, in the low level metastable unresolved picture, for He-like Ni^{26+} (in the 15-18 Angstrom) range to

adf15/transport/transport_llu#ni26ic.dat

The source adf04 is the R-matrix *adf04/helike/helike_adw05#ni26.dat*.

D.27 Add Cr^{21+} and Mn^{22+} to the *copsm#li* set. Only transitions from the lowest three levels (ground and 1s2 2p) to 1s2 nl (n=2-5) are included, following Sampson and Zhang data.

D.28 Fixed typo in:

adf18/a17_p208/exp96#li/exp96#li_c3ls.dat

to stop potential code crash; has no affect on PECs produced by ADAS208

D.29 Add charge exchange data and derived coefficients from the UAM collaboration into central ADAS.

Assessed adf01 dataset for neon: *adf01/qcx#h0/qcx#h0_uam#ne10.dat* Low energy semiclassical calculations are merged with high energy modified CTMC with special attention given to merging zone around 30-40keV/amu.

Data for Ar18: *adf01/qcx#h0/qcx#h0_uam#ar18.dat*. Improved CTMC results for n>10 are matched to ORNL CTMC results for lower n. Assessment by Hugh.

Ar17 CTMC from ORNL added to the existing Ar16 and Ar18 datasets as *qcx#h0_ornl#ar17.dat*.

Following discussions on where to archive the extracted adf01 (from Adam Foster's universal parametrisation of format adf49) data and their accompanying adf12 datasets, we have tried to keep as close as possible to the current set-up but wanted to separate the 'extracted' adf01 from assessed datasets. Therefore the following adf01 datasets have been added:

adf01/ext#h0/arf07#18/ext#h0_arf07#ar16.dat
adf01/ext#h0/arf07#18/ext#h0_arf07#ar16_n2.dat
adf01/ext#h0/arf07#18/ext#h0_arf07#ar17.dat
adf01/ext#h0/arf07#18/ext#h0_arf07#ar17_n2.dat
adf01/ext#h0/arf07#18/ext#h0_arf07#ar18.dat
adf01/ext#h0/arf07#18/ext#h0_arf07#ar18_n2.dat

which allows for per element directories – since for example W could be large. This avoids swamping the assessed data while pointing to the fact that the data has been extracted from a universal source. It also allows updating to new adf49.

Also we will have:

adf12/qef07#h/arf#18/qef07#h_arf#ar16.dat
adf12/qef07#h/arf#18/qef07#h_arf#ar16_n2.dat
adf12/qef07#h/arf#18/qef07#h_arf#ar17.dat
adf12/qef07#h/arf#18/qef07#h_arf#ar17_n2.dat
adf12/qef07#h/arf#18/qef07#h_arf#ar18.dat
adf12/qef07#h/arf#18/qef07#h_arf#ar18_n2.dat

all generated with ADAS316. These are not a perfect mirror of the adf01 directory structure but fit better with the existing collection.

All best wishes for Xmas and the New Year.

Appendix OPEN-ADAS & CXSFIT title and contents pages

OPEN-ADAS Version 1.0
Final Report

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

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Contents

CXSFIT
User Manual

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