Jan16-13 **ADAS Bulletin**

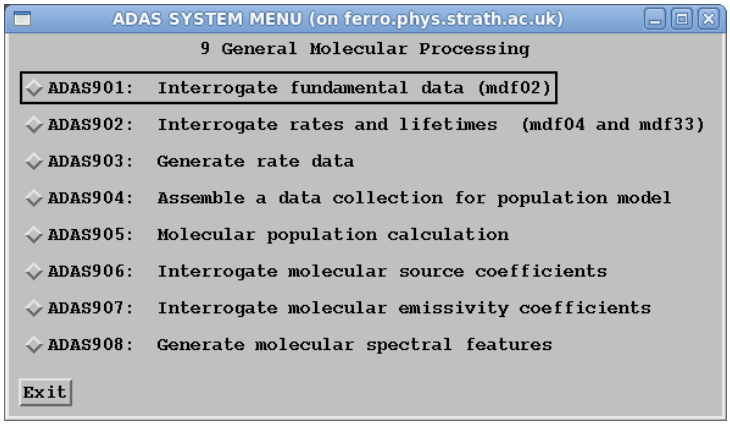
Items:

1. Introduction
2. ADAS release v4.0
3. Travel and dissemination visits in 2013
4. Next ADAS developments
5. Code and data updates in release v4.0.

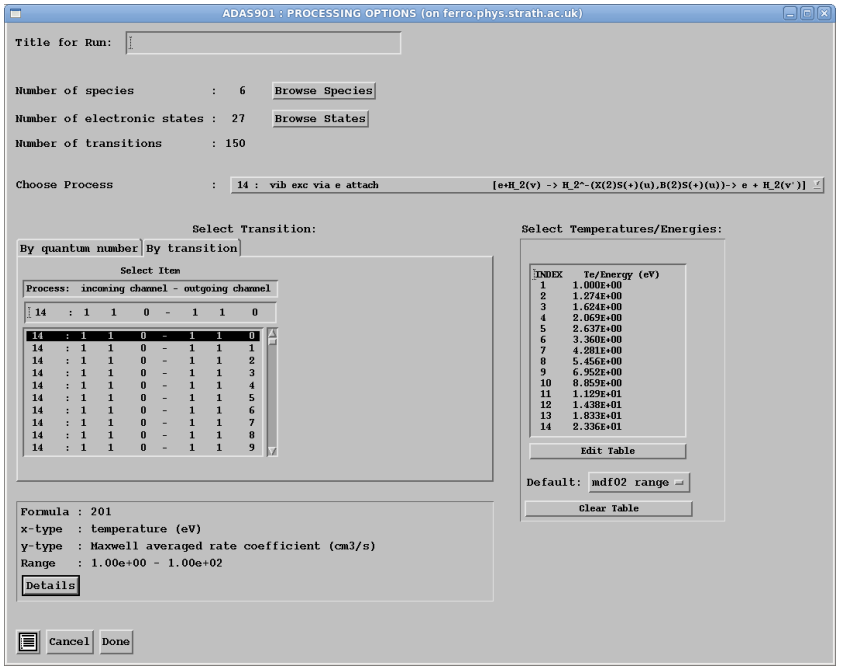
1. First of all, I should like to welcome new ADAS members, the University of Texas at Austin (William Rowan is the representative on the ADAS steering committee) and the Institute of Plasma Physics - EAST at Hefei (Juan Huang is their representative), since the last bulletin. I also note that our Russian link has now moved to the ITER Domestic Agency in Moscow (Sergei Tugarinov is their representative). We look forward to a long and fruitful collaboration. It has been rather a longer gap than usual since the last ADAS release and bulletin. However, as is evident below, release v4.0 is enormous, including nearly 10 Gbytes of new data, powerful code and method developments for offline adf04 data production and substantial extension to the spectral fitting and analysis capabilities of ADAS. It also includes the first code and data of series 9 – for molecules, a big new step for ADAS. Most of this results from the ADAS-EU Project and its ramifications. ADAS-EU completed its four-year programme on 31 Dec 2012, during which time virtually all of the main themes of ADAS, heavy species, generalised collisional-radiative modelling, ionisation state, charge exchange and beam spectroscopy, special feature spectral analysis etc, have been extended and refined. Some of these enhanced capabilities have already appeared in earlier releases, but the finalising of the main body of development has been taking place in 2012 for completion early in 2013. To get this material into play is a substantial task. It is intended to follow this release quite quickly with the next one, around mid 2013 in association with a training programme. More details are given in sections 3 and 4.

   The completion of the main body of the ADAS-EU Project means that we have had some movement of staff. Francisco Guzman has remained in France working between CEA Cadarache and the University of Marseille on a new tokamak transport/atomic physics linked project with Yannick Marandet. He expects to continue with some of his ADAS interests in molecular collisional-radiative modelling and associated connections with Integrated Atomic Modeling in Europe. Luis Menchero has remained with the University of Strathclyde, but has moved up to Glasgow to work with Nigel Badnell on the fundamental electron collision data. Alessandra is remaining with the ADAS Project, based jointly at Culham Laboratory and Rutherford Appleton Laboratory. Martin and I remain much as usual with Martin carrying the main body of ADAS support and me continuing to work in semi-retirement.

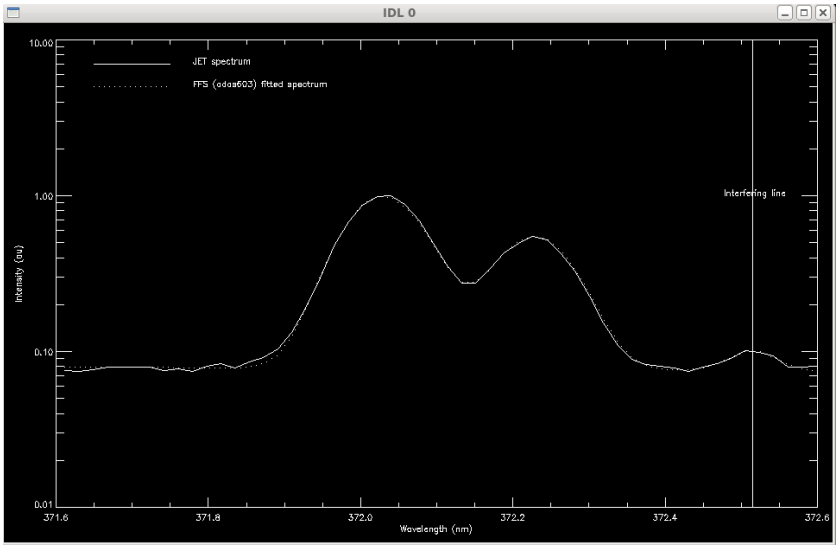
2. The menu list for series 9 is shown below. The present release is concerned only with the H_2 molecular system and includes only the first interactive code, *ADAS901*, for interrogation of molecular data format (mdf02). Note that for molecules mdf formats replace the usual adf formats for atom and ion data. mdf02 is the fundamental data class for molecular reaction cross-sections. The preparation and update of these data for ADAS has been a considerable task carried out by Fancisco Guzman, advised by Ratko Janev. There are separate datasets for electron and induced reactions and data for H_2 and H_2^+.



The file selection screen for *ADAS901* follows the usual ADAS form, but the processing screen is more elaborate than one is used to from the atom ion case. There are many different types of process and each of these is distinguished by species, electronic state and vibrational state in the incoming and outgoing channels. Collisional-radiative modelling in series 9 is at vibronic resolution. An illustrative processing screen is shown below. The ADAS vibronic collisional radiative model of the H_2 molecular system is undergoing final checks and the associated graphical user interface codes *ADAS902*, *ADAS903*, ADAS904 and *ADAS905* are in preparation for the next release. We would like to receive feedback on your impressions of *ADAS901* as we complete these other codes.



Following ADAS adf-number precedents, mdf00 is assigned to reference molecular data in various sub-directories, such as Franck-Condon factors for H_2. mdf00 for H_2 is also released now. Incidentally, mdf04 (still to be released) is the molecular equivalent of the specific ion adf04 datasets, and such datasets are sufficient to support a molecular vibronic collisional-radiative model. I also mention at this point that we are concerned to take molecular ADAS up to comparison and analysis of molecular spectra, which requires ro-vibronic resolution of spectral lines. Kurt Behringer is leading on the assembly of the rotational sub-structure models. ADAS908 will be the graphical interface to these models and their comparison with experimental data. Its preparation for the ADAS/IDL screen system is well underway and will also ready for the next release.



Some time ago, the first part of the ADAS integrated special feature handling system, called the ADAS Feature Generator (*afg*) was released, associated with *ADAS605*. This development, led by Christopher Nicholas is now complete and the second part, the Framework for Feature Synthesis (*ffs*) is now released. The combination is a sophisticated, object-oriented system, coded in IDL, for preparation of special features and then their constrained fitting to observed spectra. This package is not simple and we shall be be devoting time to it in the 2013 training courses. As a taster, some examples of its use have been placed in */home/adas/examples/afg-fss/*. The illustration above is from one of these *fit_zeeman.pro*. This is a convenient point to draw further attention to the /examples directory. You will notice sub-directories */fortran*, */idl* and */python*. We shall make increasing use of examples placed in them to guide command-line use of ADAS routines and procedures. Incidentally there is now a */home/adas/python/* library of ADAS routines.

I wish now to turn to the developments in electron collisional data and their production for ADAS. Nigel Badnell has extended the AUTOSTRUCTURE code to calculate distorted wave electron-impact excitation cross-sections as well as Plane-wave Born cross-sections. It is available in the off-line ADAS code directory */home/adas/offline_adas/adas7#1/as24*. This code allows a substantial lift of the ADAS adf04 database from plane-wave Born (*pwb*), as used extensively with the Cowan code (ADAS8#1) in ADAS, to distorted wave (*dw*). It is suited to mass production. We have moved rapidly to exploitation of *dw* with a complete machinery in the directory */home/adas/offline_adas/adas7#3/*. Recall that ADAS uses driver datasets in various sub-directories of format adf27 as input to AUTOSTRUCTURE. We have focussed on medium-weight elements between sodium and zinc in ionisation states up to argon-like for this release and their drivers are to be found in */home/adas/adas/adf27/dw* (there are also plane-wave Born drivers for AUTOSTRUCTURE in */home/adas/adas/adf27/pwb)*. These are prepared from templates which are co-located with the drivers. Scripts in */home/adas/offline_adas/adas7#3/scripts* expand the templates into individual drivers for each ion. Further scripts then execute the AUTOSTRUCTURE calculations and assemble the results in ADAS adf04 datasets. All this is conveniently done in distributed processing over many nodes. It is these datasets which have so expanded the ADAS database in this release. At this point I should say a little more about adf04. ADAS format adf04 occurs in various types (1-5). Types 1 and 5 have collision-strength transition lines, type 3 is Maxwell-averaged collision strength transition lines, while type 4 is non-Maxwellian averaged collision-strengths. Type 3 is the usual sort and if an adf04 dataset is not explicitly named with its type (such as *_t5*) then it is type 3. AUTOSTRUCTURE *dw* produces type 5, while AUTOSTRUCTURE *pwb* and Cowan *pwb* produce type 1. A separate code, included in the *ADAS7#3* scripts, converts to type 3. When you explore the adf04 mass production, note that the directory prefix *cophps* has been used and calculations are done in LS-coupling (*ls*) or intermediate coupling (*ic*). The latter is of course more suitable for medium-weight and heavy elements. So the type 3 dataset in intermediate coupling for the nitrogen-like ion Al^{+6} is */home/adas/adas/adf04/cophps#n/dw/ic#al6.dat*. There is a lot more to say about

AUTOSTRUCTURE and ADAS with respect to neutral and near neutral ions, dielectronic recombination for complex ions in the configuration average and hybrid approximations and so on which we are adding steadily to ADAS, but it requires much more guidance and explanation than is possible in this bulletin, so I simply refer on to section 3 and 4 at this point.

In this release, new generalised collisional-radiative (GCR) data are included in formats adf11, adf13 and adf15 for silicon. These are the first output of a substantial new effort on GCR which was added as an extra theme in ADAS-EU, led by Alessandra Giunta. There are a number of aspects to this. Exploitation of AUTOSTRUCTURE *dw* for level 1 and 2 collisional data completion has been referred to earlier. A second aspect is the automated preparation of ionisation rate coefficient data (ADAS format adf07) in the metastable resolved picture. This has been implemented by Alessandra (see item C.20 in section 5 below). As we move from light element GCR to medium-weight element GCR, it is necessary to change from an *ls* viewpoint with metastable terms to an *ic* viewpoint with metastable levels. The ground work for this is now nearly complete. For some time, dielectronic data in format adf09 has been prepared in *ic* resolution (see items D.12 and D.13 of section 5) with isoelectronic sequences complete up to aluminium-like. For these more complex systems, the adf09 datasets are becoming excessively large. The answer is the new hybrid adf09 datasets which Nigel Badnell has developed. These include a greater measure of level bundling while maintaining *ic* resolution for metastables. For the completion plans for medium-weight GCR, I refer forward to section 4. As a final comment here, and to show that we have not forgotten astrophysics, note that Alessandra has been reworking the differential emission measure code ADAS601, an improved version of which is included in this release. Associated studies of the solar lower chromosphere have used this method and have assisted in validating, inter alia, oxygen and silicon GCR data.

A number of other researchers have contributed important data for this release. I mention data for the ionisation state of tungsten from Thomas Pütterich. Also, we are very grateful for high-quality R-matrix data from the Auburn/Rollins team and their colleagues who include Stuart Loch, Don Griffin, John Ludlow, Dario Mitnik, Brendan McLaughlin, Teck-Ghee Lee and Connor Ballance. Guiyan Liang, now back home at the National Astronomical Observatories, CAS, in Beijing, is a major contributor. I note also beam emission corrections (see item D.15 of section 5) from Ephrem Delabie and dielectronic data from Sh. A. Abdel-Naby at Western Michigan. Also we have lots of new data from ADAS-EU specialists in Europe including Alfred Mueller, Steffan Shippers, Katarina Igenbergs, Pavel Bodganovitch, Clara Illescas and Jaime Suarez as well as from our own ADAS-EU staff Luis Menchero, Francisco Guzman and of course Nigel Badnell and Alessandra Giunta. Most of their data and its consequences for ADAS derived data we shall put out in the mid-2013 release – see also sections 3 and 4 below.

3. I wish to outline our expected travel associated with ADAS and ADAS-EU over the next nine months. The original terminal date of ADAS-EU was 31 Dec. 2012, however there is a modest underspend and the European Commission has agreed to extend the project for nine months to allow delivery of further short courses for ADAS training and knowledge transfer. Also Euratom is keen that this should support atomic physics for fusion not only in Europe and for ITER, but also worldwide including the international ITER domestic agencies. The plan is for a team of three of us, Hugh Summers, Martin O'Mullane and Alessandra Giunta to make eight visits, each of three days - four in Europe and four outside Europe - by the end of September 2013. I envisage a format somewhere between a small meeting, workshop and training course in which we would discuss local atomic physics for fusion objectives, present lectures on the advanced ADAS topics and capabilities alluded to in this bulletin, give demonstrations which show ADAS in action and finally have planning discussion with a view to long-term closer collaboration. I expect the visits to take place monthly starting with a trial one at EFDA-JET in February and an international one in Beijing in March. Possible locations, based partly on countries where an ADAS visit is overdue, are (JET/Culham, China), Russia, Japan, Korea, Juelich, F4E Spain, ITER/CEA Cadarache. The USA is certainly due a visit, but since we have many members there and various interests both astrophysical and fusion, a separate plan might be appropriate for the USA late in 2013. I should be grateful for thoughts and views on this and where we should go. I shall make up a

visit/course outline shortly for discussion. Actual content in terms of lectures and demonstrations can be adjusted according to local interests. I note though that the principal ADAS-EU documents, PUBL1-PUBL6, on the main atomic physics for fusion themes will be completed and available in time for the visits. These are large works, each covering theoretical background, code descriptions, fundamental and derived data specifications combined with the practical guidance and illustrations of a manual. Lectures, and demonstrations hopefully, should have their knowledge basis and extended study support in these documents.

4. As is perhaps evident from section 2, the efforts of the additional staff and sub-contracting from ADAS-EU has rather overwhelmed us with riches. The task for 2013 is to get all this fully in place within ADAS along with sufficient training to make full use of it. The training aspect, I have referred to in section 3. In broad terms, we shall complete the H_2 molecular work in the 1st quarter of 2013. The extension of the GCR machinery, including *ic*, with delivery of elements up to argon (possibly iron) will be completed by the end of the 2nd quarter. The 3rd and 4th quarters of 2013 will be committed to charge exchange and beam emission. I have referred to the extensive new charge exchange and ion excitation data which has been generated, but not to the sophisticated non-perturbative solution of the hydrogen atom in a Stark field (using the complex rotation method) which we now have working. This is Luis Menchero's tour-de-force and we wish to exploit the true resonance wave functions fully as part of our advanced beam emission modelling.

5. The list of code and data updates in v4.0 follows:

Corrections and updates to code (ADAS v3.1 to ADAS v4.0)

C.1 This update is ADAS v4.0 since it adds the new ADAS series 9 − General Molecular Processing.

The series 9 menu introduces the naming of the codes, many of which will be added in the course of 2013. The fundamental collision data exploration code, *ADAS901* and its associated data, archived in *adas/mdf02/h2/* is the lead code provided in this ADAS release.

C.2 When *read_adf04.pro* was changed to return the rates and effective collision strengths interpolated onto the user supplied temperatures, the excitation and de-excitation rates were returned correctly but the gamma was not. This has been corrected.

C.3 Add IDL versions of the exchange classical impact parameter (ECIP) method for electron and ion impact excitation cross-section and rates. *cxeiqp.pro* returns the cross section with *cxcrip.pro* for the excitation and de-excitation rates.

C.4 The IDL function, *xxeiam.pro*, which returns the atomic mass when the element symbol is given, has been vectorized.

C.5 In *ADSS810* the specified ion temperature is used to form the feature PEC. If the user would like Tion to be set to the electron temperature then Tion should be so specified in the adf42 driver file (or in the processing panel). Both the interactive and offline versions of adas810 have been updated.

C.6 In the *ADAS305* Stark feature code, *adas305_get_stark.pro*, and the stark feature in *ADAS603* the vacuum to air wavelength correction contained an error in one of the coefficients. The effect was to introduce a shift of ~0.3A at the H-alpha wavelength.

C.7 The matlab *read_adf* routines have been overhauled a little and should now work in a 64-bit environment. As matlab is not widely used within ADAS please contact us if there is a problem running these routines at your site.

C.8 *xxdata_40.for* reads in the comments at the bottom of the file but failed to check whether there were more than the array would hold. The routine has been fixed.

C.9 The *adas_writefile.pro* utility file can now write more than 32767 lines to the output file.

C.10 The *i4indf.pro* routine, which finds the nearest index for a value in an array has been vectorized. ie. *print, i4indf(arr, [34.5, 3, 65.0])* will now work as expected.

C.11 A significant reworking of *xxdata_04.for* to add functionality and improve validity checking of adf04 files:

- extend to accept type-4, collision strength pairs for upward and downward transitions.
- extend to accept type-5, the distorted wave collision strengths produced by autostructure. Convert to type 3 with *ADAS7#3*.
- extend to support type-6, the driver file for BBGP calculations.
- accept negative Bethe limits to identify strong dipole transitions in line with autostructure usage.
- more robust checking of the levels and transition indices.
- introduce 'T' line to denote 3-body recombination.
- introduce 'L' lines for dielectronic recombination satellite rates.

xxdata_04.pro and *read_adf04.pro* have been updated in line with these changes.

Note that although the argument list remains unchanged the checks to identify a valid adf04 file are more stringent.

C.12 The more stringent conformity check of *xxdata_04* exposed an error in the production of the configuration average adf04 files. The orbital energies line had an extra space. *adas8xx_create_ca_adf04.pro* has been updated to fix this problem and all existing datasets have been corrected.

C.13 Correcting the orbital energies exposed a limitation in *cfg2occ.pro*, the routine which converts a configuration string to an array of occupation numbers.

C.14 *ADAS414*, the soft X-ray filter generation program now offers all of the elements in Henke's database. Previously only a subsection was offered since the GUI droplist moved off the bottom of the screen. The GUI has been altered to ease selection from a longer list.

Related updates, since the element platinum (Pt) has 8 edges:

- *read_adf35.pro* will now read adf35 files which have 10 edges, up from 5.
- include the same increase to 10 edges in *ADAS408*.

C.15 In *ADAS801*, the Cowan code, more control on the number of configurations included in the adf04 file has been enabled.

In some applications not all the configurations required for the structure calculation, eg when including extensive configuration interaction effects, are required for the population calculation. By reducing the number of output configurations the size of the calculation, and resources needed, are much reduced without compromising the improvements in the structure.

In a related development the core-polarization (HFR+CPOL) method of the Astrophysics and Spectroscopy (ASPECT) group of Mons University (Belgium) extra input files to the *run_adas8#1.pl* perl driving script. We have found that limiting the number of configurations in the adf04 file can be become essential in these cases.

In the interactive *ADAS801* the configurations are selected via the 'Extra options....' button. In the offline perl script they are specified in the instruction and post-processing files. Note that the adas801 defaults has extra information so the existing one will need to be deleted.

When the Eissner form of the configurations is selected the leading 5 for the first shell is retained. Previously it was dropped but keeping it as a triplet conforms better to the original definition.

We have taken this opportunity to use the same code for the interactive and offline versions of the Cowan code. The offline version will be installed and compiled as part of the standard ADAS

release. Note that this does not affect the ability to run the offline code on machines other than the ADAS installation. There is no dependence on IDL but a fortran compiler and perl are required.

C.16 In *ADAS208* when writing CX PECs for the un-normalized, metastable resolved case, a check was added to set a minimum value of 1.0e-74. Unfortunately this check was inverted resulting in all entries being written as 1.0e-74.

The default behaviour for normalization in *run_adas208.pro* is to switch it on, which is the mode most usually wanted. The keyword chosen to change this was named 'norm' but the check was not performed correctly. Therefore the keyword has been changed to nonorm to make selecting this mode an active choice: if */nonorm* is set (or *nonorm=1*) then normalization is not applied. If this keyword is omitted (or by setting *nonorm=0*) no normalization is applied.

C.17 In *ADAS404* incorrect units (cm3/s rather than Wcm3) were written to the comment section of the metastable un-resolved prb and prc adf11 files. The metastable resolved versions (*prbYYr/*) were correct.

C.18 The *xxcftr.for* routine for converting configurations between standard and Eissner forms has been updated to permit longer length configurations and to accept Eissner forms composed of sets of triplets or a leading doublet followed by triplets. ie 563514515 is valid and is the same as 63514515, or 2p6 3s1 3p1 for the uninitiated.

C.19 *ADAS407* was updated to incorporate the longer configurations permitted by *xxcftr* and the opportunity was taken to fix a number of small bugs. A new *run_adas407.pro* routine has been added to allow scripting of adf03 generation and operates on pairs of adf04 files. Note that *ADAS407* also produces the input file for *ADAS204*, of adf25 type and *run_adas407.pro* can optionally create these, although some minor subsequent editing is required.

C.20 One of the more esoteric, and hand worked, parts of the GCR workflow has been automated. Metastable resolved ionisation rates are required for the adf04 files (S-lines) but often just unresolved, zero density, ionisation rates are available (adf07 and adf23 collections). These total rates are split according to the spin system weights. The ionisation potentials and term energies between the metastables are taken from adf04 files. The procedure becomes complex when more than a ground+metastable set are involved. The new routines:

idl/adaslib/proc_adf/pathways_adf07.pro
idl/adaslib/proc_adf/fractionate_adf07.pro

set up the pathways and write the driver file for the *split_adf07.pro* routine. Iso-electronic sequences up to Fe-like can be used.

Some support routines, of general interest, have been added:

idl/adaslib/atomic/xxterms.pro - returns all possible terms for a given configuration
idl/adaslib/atomic/xxorbocc.pro - returns the occupation number for an orbital.

C.21 *ADAS601*, the differential emission measure (DEM) analysis code has been adjusted to improve extrapolation at low temperatures in order to improve the convergence of the model. Units for the intensity should now be supplied in the input file, although the code will default to photons if they are not present. The example files in */home/adas/arch601/intensity/* have been changed.

The documentation has also been updated with references to Astronomy and Astrophysics journal articles.

C.22 Some adf04 files contain a large number of energy levels and transitions. In particular the intermediate coupled, distorted wave, baseline data in *adf04/cophps#<seq>/* contain inner shell excitation which can result in many energy levels above the ionisation potential for lower Z members of the sequence. The size of the dataset can overwhelm the population codes.

An IDL routine,

idl/adaslib/proc_adf/trim_cophps_adf04.pro

can be used to reduce the size of an adf04 file by retaining those energy levels (and associated transitions) below a user set threshold. The default is 105% of the ionisation potential.

Despite its name this routine can be applied to any adf04 file. It has an additional option to replace the Eissner notation, in the DW corpus and the heavy species *adf04/coparf#<Z>* files, with a standard configuration nomenclature.

write_adf04.pro required a slight adjustment to work with this routine.

C.23 The latest version of AUTOSTRUCTURE has been added to *offline_adas/adas7#1*. It can be run from the executable

../offline_adas/adas7#1/bin/as24.x

with code in

../offline_adas/adas7#1/src/as24/

Note that the previous version distributed with ADAS was v18.14. This has been retained in

../offline_adas/adas7#1/src/

to allow reproduction of previous results, particularly adf09 DR data.

Newer versions will be released in *offline_adas/adas7#1/as<VER>* directories.

As with the adas8#1 offline_code the compilation is now integrated into the main ADAS build system. A file,

../offline_adas/adas7#1/make_adas7#1

is driven by a central choice of compiler (to permit multiple site compilation). However it can be used in a stand-alone scenario by defining the

COMPILER - compiler fortran
EXTRAFF - flags for compiler
LINKER - linker
LIBS - external libraries

C.24 A new offline_adas code, *ADAS7#3*, is introduced to enable the mass production of distorted wave (and plane wave Born if required) adf04 data. Both cross section and Maxwell averaged effective collision strength versions are produced.

AUTOSTRUCTURE (*ADAS7#1*) is the fundamental physics code and *ADAS7#3* provides a complete set of scripts for generating the input drivers, assembling these by iso-electronic sequence and post-processing the output to an adf04 type 3 delivery.

To convert between type 1 or type 5 (cross section) to type 3 (standard Maxwellian effective collision strengths) use

../offline_adas/adas7#3/bin/adf04_om2ups.x

generated from

../offline_adas/adas7#3/fortran/adf04_om2ups.for
../offline_adas/adas7#1/make_adas7#3

Note that this (unix) command line program can be optionally supplied with input and output files as arguments. It assumes that these are *adf04_om* and *adf04_ups* respectively if not given.

Note that the *adf04_om2ups* post-processor can take as an optional input an adf37 file with a numerical electron energy distribution function. This generates a type 4 adf04 file which is designed for non-Maxwellian population modelling.

The perl scripts, in *../offline_adas/adas7#3/scripts/*, are run in sequence as

1. *setup_isoseq_pwb_adf27.pl*

   - this script sets up the adf27 driver files for AUTOSTRUCTURE based on a set of template files (generated by hand)
     <adasroot>/adas/adf27/pwb/<seq>like/<userdircode>#<seq>/template

- user set arguments are:
  -- *adasroot=/home/adas* for central ADAS version but can be user's copy of code
  -- *userdircode=cophps* baseline mass production name
  -- *isoseq=na* sodium-like sequence example
  -- *element_category=light* set of light elements (*medium* or *heavy* are allowed).

  optional, these defaults to adasroot if not set

  --*indir=/home/abc* non-adasroot location of templates
  --*outdir=/home/abc* non-adasroot location of adf27 drivers

2. *process_ion_pwb_adf27_to_adf04.pl*

- runs AUSTOSTRUCTRE (*ADAS7#1*) to generate IC and LS plane wave Born adf04 files of type 1. Runs *adf04_om2ups.x* to convert to type 3.

- user set arguments are:
  --*adasroot=/home/adas* for central ADAS version but can be user's copy of code
  --*userdircode=cophps* baseline mass production name
  -- *isoseq=na* sodium-like sequence example
  --*ion=s5* Sulphur S+5

  optional, these defaults to adasroot if not set

  --*indir=/home/abc* non-adasroot location of adf27 driver
  --*outdir=/home/abc* non-adasroot location of adf04 pwb

3. *setup_isoseq_dw_adf27.pl*

- this script sets up the adf27 driver files for AUTOSTRUCTURE based on a set of template files in central ADAS
  <adasroot>/adas/adf27/pwb/<seq>like/<userdircode>#<seq>/template
  and the set of plane wave Born adf04 datasets (steps 1+2).
- user set arguments are:
  --*adasroot=/home/adas* for central ADAS version but can be user's copy of code
  --*userdircode=cophps* baseline mass production name
  --*isoseq=na* sodium-like sequence example
  --*element_category=light* set of light elements (*medium* or *heavy* are allowed).

  optional, these defaults to adasroot if not set

  --*indir=/home/abc* non-root location of IC and LS template files
  --*outdir=/home/abc* non-adasroot location of adf27 drivers
  --pwbdir=/home/abc non-adasroot location of PWB adf04 files

4. *process_ion_dw_adf27_to_adf04.pl*

- runs AUSTOSTRUCTURE (*ADAS7#1*) to generate IC and LS distorted wave adf04 files of type 5. Runs adf04_om2ups.x to convert to type 3.

- user set arguments are:
  --*adasroot=/home/adas* for central ADAS version but can be user's copy of code
  --*userdircode=cophps* baseline mass production name
  --*isoseq=na* sodium-like sequence example
  --*ion=s5* Sulpher S+5

  optional, these defaults to adasroot if not set

  --*indir=/home/abc* non-adasroot location of adf27 driver

--outdir=/home/abc non-adasroot location of adf04 dw

Two further scripts are provided:

adas7#3_dw_llbatch.pl

adas7#3_pwb_llbatch.pl

These scripts were used to run the above steps for each sequence under the JET loadlevellller system are included as guidance to porting the system to a different batch job scheduler.

C.25 A python library has been added. This is modelled on the IDL library and makes extracting ADAS data and selected codes and routines available to python programs. These may also be called from the python command line (or the ipython environment).

It will be necessary to add the ADAS python library to the PYTHONPATH environment (bash and csh):

export PYTHONPATH=:/home/adas/python:$PYTHONPATH

setenv PYTHONPATH ":/home/adas/python:$PYTHONPATH"

As with IDL the python library starts modestly with routines being added as needed.

With numpy and f2py now mature, and more importantly widely available, we have a reasonable expectation that the system to support the ADAS python library will be available at all ADAS sites. Or it can be easily installed from standard distribution repositories.

The first steps were to choose a number of routines to test the feasibility and to incorporate the compilation and packaging of the library into the ADAS build system. The routines chosen are

xxdata_12:	Returns all the data in an adf12 CX effective emissivity coefficient file.
xxdata_21:	Returns all the data in an adf21 beam stopping (adf21) file.
read_adf12:	interpolates/extrapolates a CX emissivity coefficient (adf12) onto a user supplied energy/temperature/density/ Zeff/Bfield set of parameters.
read_adf21:	interpolates/extrapolates onto a user supplied set of energy/Te/density a total effective beam stopping coefficient made up from a number of elements.
cxsqef:	Underlying extraction routine for read_adf12.py but with more user control.
read_adf15:	interpolates/extrapolates a photon emissivity coefficient (adf15) onto a user supplied Te/density set of pairs or grid.
run_adas405:	Solves the equilibrium ionisation balance (and radiated power) onto a user supplied Te/density set of pairs or grid. adf11 year numbers or files can be specified.
stark :	Returns the components of the Stark spectrum for a user supplied set of beam, plasma, E/B field and observation parameters.
c5dplr:	Doppler broadens a set of discrete emissivities, such as a Stark manifold.
adas_vector:	returns a default log spaced vector

These were chosen to reflect current interests and to examine the different ways that the python code can be integrated with the underlying ADAS fortran code. run_adas405 interacts via a bi-directional pipe, just like the IDL run_adas405.pro version, whereas the others build a .so shared executable with f2py in an analogous way to IDL's call_external method. The fact that a lot of glue/wrapper code for fortran-IDL is available has made this simpler, although it is not a fully automatic process as the f2py signature files need to be modified a little.

C.26 IDL routines, extracted from *ADAS309*, are provided to calculate charge exchange driven effective emissivity coefficients directly from the adf01 cross section files without the interpolation step of reading from an adf12 dataset. These are useful if the adf12 reference conditions are not appropriate.

c9cxee.pro provides the most control and evaluates the QEF at one set of plasma/beam conditions (note that the adf01 data must be pre-processed with calls to *cxfrac.pro* and *cxextr.pro*).

adas309_qeff.pro provides a convenient way to extract QEF data along a profile by packaging these steps. Note that *run_adas308.pro* provides this capability but *adas309_qeff.pro* is much more efficient.

C.27 The Framework for Feature Synthesis (*ffs*) an object oriented model and fitting library is available in ADAS v4. Based on the PhD work of Chris Nicholas it is a comprehensive framework for constrained fitting of observed spectra to ADAS feature; these features can be simple or super features and range from isolated lines to Zeeman-split multiplets and feature PECs (adf40). Backgrounds, line profiles and multiple features can be combined in the fit.

The features are accessed via the ADAS feature Generator (*afg*) library which has been in ADAS for some time, and which powers the *ADAS605* interactive exploration program.

Note that both *afg* and *ffs* are implemented in IDL.

C.28 The promote use of ADAS codes outside the interactive system a new examples directory containing heavily commented routines demonstrating the use of ADAS prodeures (and data) in fortran, IDL and python. The fitting of a JET BeII spectrum, split by the magnetic field, using *ffs* methodology, is given.

We hope this will evolve into a cookbook for ADAS code use and would welcome code which demonstrates all aspects of ADAS use.

Corrections and updates to data (ADAS v3.1 to ADAS v4.0)

D.1 The ionisation potentials in the adf00 datasets for second and third row elements have been updated using NIST (v4.0) values by Adam Foster. The lighter elements, along with Mg, Si,Fe and W were already up to date. Data for the remaining elements may take some time to find.

The resolved adf00 data set variants, <elem. symb>_ls.dat and <elem. symb>_ic.dat, up to iron have been included. The first line of the format has been modified to allow a "wf=" entry. This denotes a "work function" which is appropriate for precise usage with *ls* resolution metastable terms. It is the energy of the lowest metastable above the true ground energy. The ionisation potential is then that of the lowest metastable term.

xxdata_00.for and *read_adf00.pro* have been updated to use the new format.

D.2 Some existing adf04 files were found to contain errors:

copmm#9/ls#f0.dat:	The file was not neutral fluorine and has been replaced.
copmm#36/ls#kr8.dat:	The ground level had an incorrect Eissner label.
copmm#36/ls#kr9.dat:	Level 19 had an incorrect Eissner label.
copmm#28/ls#ni1.dat:	Level 54 had an incorrect Eissner label.
helike/helike_ihc90cl.dat:	Incorrect terminators.
hlike/hlike_mom93#he.dat:	Bring into line with adf04 specification.

D.3 Some other minor corrections to adf04 files, which do not merit a new dataset.

adas#10/cop98#10_ls#ne4.dat:	2S1 2P2 3S1 was listed as 2S2 2P2 3S1, that is with one electron too many.
adas#10/cop98#10_ic#ne4.dat:	ditto

D.4 The orbital energies, particularly, in the coparf#<Z> heavy species adf04 files, did not follow the adf04 specification. Orbitals not present in the set of configurations should be given as 0.0 in the

strictly hydrogenic orbital data line. The rules restricting the change in l-quantum number used to limit the size of these datasets means that this set of data was more compromised than the main body of adf04 data.

The argon and tungsten (coparf#18 and coparf#74) datasets have been corrected.

In addition to these a small number of other adf04 files were found to be in error. The following have been also been corrected:

adas#6/mom97_ls#c0.dat
clike/clike_cfm96#c.dat
clike/clike_mom97#c0.dat
clike/clike_rhgr93c.dat
copss#li/copss#li_ss#o5j.dat
lilike/lilike_wjd91be.dat

copmm#6/	c0	
copmm#7/	n 0-5	
copmm#17/	cl14	
copmm#26/	fe13-14, 16-22, 24	
copmm#28/	ni2-7, 11, 15, 16, 18-24, 26	(see above for ni1)
copmm#36/	kr8-10, 15, 16, 18, 19	
copmm#42/	mo0-3	
copmm#54/	xe0-5, 9-17, 27-34	

D.5 A set of adf11 data for tungsten, assembled by Thomas Pütterich and used for analysis at Asdex Upgrade has been added to ADAS. The year/token naming is extended by assigning the year '50' to data originating rom AUG.

Four datasets are available:

scd50/scd50_w.dat :	original source is CADW data from Stuart Loch (Phys. Rev. A (At. Mol. Opt. Phys.) 72 052716) so there is no density dependence
acd50/acd50_w.dat :	based on ADPAK data from Post (Atomic Data Nuc. Data Tab, 20, (1977), p397) but modified by Thomas with Te-independent factors for W21+ -> W55+ (see Pütterich et al. PPCF 50 (2008), 085016)
plt50.plt50_w.dat :	Line power calculated with adas810 based on adf04 files created by Thomas.
prb50/prb50_w.dat :	Based on the acd50_w.dat data.

Discussion on the data are in Thomas's thesis available from:
http://edoc.mpg.de/display.epl?mode=doc&id=260878&col=33&grp=1311
and in subsequent papers.

D.6 Some photon emissivities (adf15) and ionisation per photon (adf13) coefficients were missing for a number of nitrogen visible lines. This is the old idiosyncrasy of *ADAS208* which used to favour the strong VUV lines over the weaker, but more easily observed, transitions in the visible.

In line with the carbon naming conventions there new vsu (visible, metastable unresolved with projection) datasets:

adf15/pec96#n/pec96#n_vsu#n0.dat
adf15/pec96#n/pec96#n_vsu#n1.dat
adf15/pec96#n/pec96#n_vsu#n2.dat

adf13/sxb96#n/sxb96#n_vsu#n0.dat
adf13/sxb96#n/sxb96#n_vsu#n1.dat
adf13/sxb96#n/sxb96#n_vsu#n2.dat

These have the same fundamental adf04 input as the equivalent pju (metastable resolved with projection) and can be considered as extensions of them.

D.7 The units reported in the comments of some adf11 PRB and PRC were incorrect. In the 96 unresolved files, the most used variant, the power was incorrectly given as a rate. The comments have been updated with the correct version. Note that the numerical data is unchanged. The affected files are:

prb96/prb96_be.dat
/prb96_c.dat
/prb96_he.dat
/prb96_li.dat
/prb96_n.dat
/prb96_ne.dat
/prb96_o.dat
prc96/prc96_c.dat
/prc96_he.dat

D.8 R-matrix excitation data for neon, from the Auburn/Rollins group, has been added to the isoelectronic sequence directories:

flike_dcg01#ne1.dat :	Donald Griffin	(1)
olike_tgl10#ne2.dat :	B McLaughlin/Teck-Ghee Lee	(2)
nlike_jal10#ne3.dat :	John Ludlow	(2)
clike_dcg00#ne4.dat :	Donald Griffin	(3)
blike_dmm01#ne5.dat :	Dario Mitnik/Donald Griffin	(4)
belike_jal10#ne6.dat :	John Ludlow	
lilike_jal10#ne7.dat :	John Ludlow	(5)
helike_jal10#ne8.dat :	John Ludlow	(5)
hlike_jal10#ne9.dat :	John Ludlow	(5)

(1) Update of the May 11, 2001 version. More detailed comments with some minor numerical differences between high lying levels (115 and above) at the high temperatures.
(2) More than 500 levels and 150000+ transitions
(3) Original central ADAS file replace with this version which extends to lower temperatures and had infinite energy limit points.
(4) Update of the June 22, 2001 version. More detailed comments with some minor numerical differences between high lying levels at the high temperatures.
(5) Not in literature but generated for ADAS to complete ionised neon set.

D.9 R-matrix excitation data for argon, from the Auburn/Rollins group, has been added to the isoelectronic sequence directories:

arlike_cpb12#ar0.dat
plike_jal10#ar3.dat
silike_jal10#ar4.dat
allike_jal10#ar5.dat
nalike_jal10#ar7.dat
nelike_jal10#ar8.dat
olike_jal10#ar10.dat
nlike_jal10#ar11.dat
clike_jal10#ar12.dat
blike_jal10#ar13.dat
belike_jal10#ar14.dat

hlike_jal10#ar17.dat

Details have been published in:
C P Ballance et al, J. Phys. B41, (2008), 065201
J A Ludlow et al, J. Phys. B43 (2010), 074029

D.10 R-matrix data for four sulphur ions, S+8-S+11, from Guiyun Liang had been added to the isoelectronic directories:
olike/olike_lgy11#s8.dat
nlike/nlike_lgy11#s9.dat
clike/clike_lgy11#s10.dat
blike/blike_lgy11#s11.dat

Details have been published in:
G Y Liang et al, Astron. Astrophys., 533 (2011), A87

D.11 Add Sampson adf04 files for H-like Al+12 and Cu+28 to *adf04/copsm#h/*.

D.12 There were some minor formatting errors in some adf09 file - extra blank lines which affected the reading routine *xxdata_09.for*. The numerical data is unchanged. The corrected files are:

- In *adas/adf09/nrboiz00#c/*

oiz00#c_al7ls22.dat	*oiz00#c_k13ls22.dat*	*oiz00#c_p9ls22.dat*
oiz00#c_ar12ls22.dat	*oiz00#c_mg6ls22.dat*	*oiz00#c_s10ls22.dat*
oiz00#c_ca14ls22.dat	*oiz00#c_n1ls22.dat*	*oiz00#c_sc15ls22.dat*
oiz00#c_cl11ls22.dat	*oiz00#c_na5ls22.dat*	*oiz00#c_si8ls22.dat*
oiz00#c_cr18ls22.dat	*oiz00#c_ne4ls22.dat*	*oiz00#c_ti16ls22.dat*
oiz00#c_f3ls22.dat	*oiz00#c_o2ls22.dat*	*oiz00#c_v17ls22.dat*

- In a*das/adf09/nrbza00#b/*
za00#b_zn25icr23.dat

- In *adas/adf09/za00#mg/*

za00#mg_ar6ic23.dat	*za00#mg_cr12ls334.dat*	*za00#mg_sc9ic334.dat*
za00#mg_ar6ic334.dat	*za00#mg_fe14ic334.dat*	*za00#mg_sc9ls334.dat*
za00#mg_ar6ls23.dat	*za00#mg_fe14ls334.dat*	*za00#mg_ti10ic334.dat*
za00#mg_ar6ls334.dat	*za00#mg_k7ic334.dat*	*za00#mg_ti10ls334.dat*
za00#mg_ca8ic334.dat	*za00#mg_k7ls334.dat*	*za00#mg_v11ic334.dat*
za00#mg_ca8ls334.dat	*za00#mg_mo30ic334.dat*	*za00#mg_v11ls334.dat*
za00#mg_cl5ic23.dat	*za00#mg_mo30ls334.dat*	*za00#mg_xe42ic23.dat*
za00#mg_cl5ic334.dat	*za00#mg_ni16ic334.dat*	*za00#mg_xe42ic334.dat*
za00#mg_cl5ls23.dat	*za00#mg_ni16ls334.dat*	*za00#mg_xe42ls23.dat*
za00#mg_cl5ls334.dat	*za00#mg_s4ic23.dat*	*za00#mg_xe42ls334.dat*
za00#mg_co15ic334.dat	*za00#mg_s4ic334.dat*	
za00#mg_co15ls334.dat	*za00#mg_s4ls334.dat*	

D.13 Dielectronic recombination data for the Al-like sequence has been added. These data were calculated by Sh. A. Abdel-Naby (Western Michigan University) and Nigel Badnell (Strathclyde) and have been reported in Astronomy and Astrophysics, vol537, A40 (2012).

The data are archived in
adf09/nrbsaan00#al/saan00#al_<elem><iz><coupling><nn'>.dat
/nrb00#al_<elem><iz><coupling><nn'>.dat
for ic and ls coupling and 3-3 and 3-4 cores.

Data added for:

Si^{+1}, P^{+2}, S^{+3}, Cl^{+4}, Ar^{+5}, K^{+6}, Ca^{+7}, Sc^{+8}, Ti^{+9}, V^{+10}, Cr^{+11},
Mn^{+12}, Fe^{+13}, Co^{+14}, Ni^{+15}, Cu^{+16}, Zn^{+17}, Kr^{+23}, Mo^{+29} and Xe^{+41}

AUTOSTRUCTURE (*ADAS701* and *ADAS7#1*) and post-processor (ADAS702) driver files are in:

adf27/dr/allike/nrb00#al/
adf27/dr/allike/saan00#al/
adf28/dr/allike/nrb00#al/
adf28/dr/allike/saan00#al/

D.14 Add two transitions (4s $^3P_2$ - 4p $^3D_3$ and 4s $^3P_1$ - 4p $^3D_1$) to the neutral argon PEC file, *adf15/transport/transport_llu#ar0.dat*.

D.15 There was a long lasting discrepancy between the measured beam emission and the calculated value from an attenuation calculation. A re-examination of the fundamental data and new experimental observations has shown that the difference is removed when corrections to some cross sections are applied. The results were reported in

E Delabie et al, Plasma Phys. Control. Fusion, vol 52, (2010), 125008.

These corrections were further improvements to the corrections made in the last ADAS release, labelled 98 (eg *bms98#h_h1.dat*).

There are new adf26, adf21 and adf22 data for hydrogen. We have used the year 10 as an identified for these, following the nomenclature in Ephrem's paper.

Data is provided for the standard plasma and beam energy conditions suited to present day beam heating and a set targeted at future high energy heating beams envisaged for ITER and DEMO. Note that only the stopping coefficients are provided but the others can be easily generated (using *ADAS312*) from the adf26 files if required.

The bundle-n tabulations are:

adf26/bdn10#h/bdn10#h_h1.dat
df26/bdn10#h/bdn10#h_fast_h1.dat

The beam stopping coefficients:

adf21/bms10#h/bms10#h_h1.dat
adf21/bms10#h/bms10#h_fast_h1.dat

The beam emission coefficients:

adf21/bme10#h/bme10#h_h1.dat

The beam excited population fractions:

adf21/bmp10#h/bmp10#h_2_h1.dat
adf21/bmp10#h/bmp10#h_3_h1.dat
adf21/bmp10#h/bmp10#h_4_h1.dat

Note that there is no change in the adf21 and adf22 data for the impurities, so the existing '97' set is still current.

D.16 Fashions change and in the summer of 2012 DEMO is favouring argon. High energy beam stopping coefficients for argon have been added to the existing '99' data

adf26/bdn99#h/bdn99#h_fast_ar18.dat
adf21/bms99#h/bms99#h_fast_ar18.dat

Note that these new 'fast'-beam stopping coefficients are stored in the same directory as the existing Ar18+ data, unlike the separate fast directory for the light elements. This is partly historic

since argon was not part of the original light element evaluation and was placed, along with iron, in its own directory.

D.17 Lithium as a first wall material is being investigated in a few tokamaks so conventional CXRS analysis may be possible. We had adf01 (cross sections) and adf12 (effective emissivities) for the n=2 hydrogen donor but nothing for the n=1 contribution. Lithium was not envisaged when the ADAS recommended data was assembled.

An adf01 dataset was extracted from the universal formula with *ADAS315* and adf12 emissivity coefficients are calculated. However this Li^{3+} data is not as well scrutinized as the other light elements and the lowest energy in the adf01 (and adf12) dataset is set to 10keV/amu, 10 times higher than the other light elements, since the trend as a function of energy for the total cross section is flat for the extracted cross section but falls strongly according to the total in *adf02/sia#h/sia99#h_j99.dat*. Above 10keV/amu the trend and turning points are in reasonable agreement.

The data is stored in the extracted collections:
adf01/ext#h0/arf07#3/ext#h0_arf07#li3.dat
adf12/qef07#h/arf#18/qef07#h_arf#li3.dat
(we acknowledge that the naming is not self-consistent).

It was discovered that the wavelength for the n=5-4 transition detailed in the comments of
adf12/qef97#h/qef97#h_en2_kvi#li3.dat
was incorrect. However the emissivity coefficient data was correct and is unchanged.

D.18 One adf48 file, the state selective radiative recombination data, had a number of NaNs in the file. The code was re-run for
adf48/nrb05#n/nrb05#n_mg5ls.dat
and the new rates were verified to be extremely small. The total rate was unchanged.

The comments of all the adf48 files were updated to include a link to the original literature reference, N. R. Badnell, ApJS, vol 167 (2006) p334.

D.19 A new set of baseline adf04 (specific ion) data has been added and substantially increases the size of the ADAS database --- by close to an extra 10Gb.

The uplifted baseline is distorted wave collision data which is a significant improvement over the plane wave Born of the previous mass production. All the data has been produced with the updated offline *ADAS7#1* and *ADAS7#3* codes which are the ADAS versions of AUTOSTRUCTURE and its post-processors.

The H-like to Ar-like isoelectronic sequences for all the light elements, hydrogen to zinc are available in term resolved (LS) and intermediate coupling resolutions. The data can be found in the directories:
adas/adf04/cophps#h/dw/
adas/adf04/cophps#he/dw/
.
.
adas/adf04/cophps#ar/dw/

The usual, Maxwell averaged, type 3 data sets are provided (eg, ic#ni10.dat, ls#cu14.dat etc.) but a type 5 specific ion file is also available (eg, ic#sc5_t5.dat, ls#na8_t5.dat). *ADAS809* can process these files with an arbitrary electron distribution functions, and given the breadth of the new data, non Maxelllian studies are no longer stymied by the lack of suitable cross section data.

D.20 A longstanding oddity in the hydrogen S/XB curves has been resolved. The curves were not smooth but had a kink at ~10eV. This was most noticeable in the SXB and, to a lesser extent in the photon emissivity coefficients but its influence could also be seen in the other GCR coefficients, ie the ionisation and recombination rates and the line power coefficient. The 96 data for hydrogen is erroneous.

The cause was traced to an oversight in assembling the excitation data which were in separate low and high temperature files. However the discrepancy arises from transitions where the excitation data was an empirical extrapolation due to the unavailability of calculated ab initio collision strengths when these files were assembled.

R-matrix with pseudo-state collision strength data is now available and is a significant improvement on the earlier work. Although the existing 96 data could be corrected it is preferable to add a new set of data which uplifts the quality of the data.

The new ADAS dataseta are:

adas/adf13/sxb12#h/sxb12#h_pju#h0.dat
adas/adf15/pec12#h/pec12#h_pju#h0.dat
adas/adf11/acd12/acd12_h.dat
adas/adf11/scd12/scd12_h.dat
adas/adf11/plt12/plt12_h.dat
adas/adf11/prb12/prb12_h.dat

Full details on the extent and consequences of this error are in the ADAS note,
adas/doc/notes/adas_c13-01.pdf.

D.21 Added ADAS molecular data class mdf00, with the following subdirectories:

/home/adas/mdf00/aval/h2/	A-values
/fcf/h2/	Franck-Condon factors
/enu/d2/, dt/,h2/,hd/,ht/,t2/	vibrational energies

aval data sets of form aval<aa><bb>-<cc><dd>.dat and
fcf data sets of form fcf<aa><bb>-<cc><dd>.dat and
fcf data sets of form enu<cc><dd>.dat where
<aa> = lower state species index , <bb> = lower electronic state index , <cc> =upper state species index , <dd> = upper electronic state index.

D.22 Added ADAS generalised collisional-radiative data in formats adf11, adf13 and adf15 for silicon. These data are under year number '96'. The fundamental specific ion files are in /home/adas/adas/adf04/adas#14. There are also supporting files in the adf08, adf10, adf17, adf18 and adf25 collections.

HPS
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