May18-05 **ADAS Bulletin**

Items:

1. ADAS release v2.9
2. The April ADAS work-in.
3. Plans for ADAS release v2.10
4. Code and data updates in release v2.9.

1. ADAS release v2.9.

There is quite a variety of material in this latest ADAS release. Since most of it is either data or concerned with running ADAS codes at the IDL or Unix command line with no screen dumps for illustration, I should draw to some of the main developments.

On codes, you will notice more attention to *read_adfxx* procedures with a /help keyword added and the new *read_adf35.pro* and *read_adf16.pro*. The latter accesses GTN functions. That is the astrophysical contribution function G(Te) but the definition of our *adf16* is a function of Te and Ne following proper collisional-radiative modelling. It does not include the solar atmosphere N_H/Ne ratio and so is more suitable for general plasma use. Note that the simpler solar G(Te) are also available in ADAS as format *adf20*. High quality GTN functions are a principal need for astrophysical analysis and (largely motivated by interest at the April work-in), Martin has been improving matters. The code ADAS408, which has been somewhat ignored (except by Alessandro) in recent years has been brought up to date with some errors corrected and *run_adas405.pro* has been extended. There is still more to do on the filtered case. More importantly Martin has provided the IDL command line procedure *adas409_generate_gtn.pro* summarised in entry C25 for automatic GTN production. We hope now to build the adf16 GTN database substantially (see item 3).

Then we have finally returned to beam attenutation and beam emission. Both Sanjay at Wisconsin Madison and Michael at TUW Vienna have been testing the developments. Mainly these include a revision of ADAS311 for helium beam modelling, rationalising the work of Harvey Anderson with central ADAS, organising the projecttion data for output by ADAS311. The situation is now stable and improved, but I think that one further iteration, including ion data improvement, is required before we can leave it and this is underway. Howevever the revised ADAS311 is released now. Also Martin has made available our ab initio Stark feature modelling as an IDL command line procedure *adas305_get_stark*. Note that we have had a place holder for Stark modelling in ADAS305 for many years but have until now not got round to bringing it up – partly due to motional Stark analysis being focussed rather on polarimetry. This release does not bring ADAS305 up as an interactive ADAS code yet but we trust that *adas305_get_stark* will be helpful.

Finally on codes note also the availability of free-free and free-bound continuum modelling, *continuo* at the IDL and Fortran levels. This is Lorne Horton's assembly of the ADAS free-free and bound-free primitives in a more usuable form. Also, further items tying up non-Maxwellian modelling – on which the final part of the story will be next release in time for the ADAS workshop.

On data, you will be aware of the large additions (and corrections) to the adf09 dielectronic data and associated drivers. The DR project has been running for some time under Nigel's guidance and is being increasingly widely used in large scale astrophysical work (albeit mostly totals). Such coordinated work requires a lot of checking and Allan has nobly given adf09 some loving care and attention, for which we are grateful. In amongst the list of DR corrections, there are quite a few things to draw attentiion to – a *.err* file for the neutral helium adf04 type 1 file and it propagation through to the *.err* file for the adf04 type 3 Maxwell average file. Also there are baseline adf04 data for copper, adf11 files for molybdenum and copper.

Finally notice that at there have been some updates to the web site.

2. The April ADAS work-in at Strathclyde.

The work-in this year was on astrophysical plasma modelling and analysis, with a strong emphasis on calculation of key additional fundamental collision data, especially electron impact excitation and ionisation data. Astrophysicists were well represented with Randall Smith (Goddard Space Flight Center), Gerry Doyle (Armagh Observatory), Alessandro Lanzafame (Catania Observatroy) Guilio Del Zanna (University College) and Peter Young (RAL). Also all our home team were present including

Stuart Loch back over from Auburn University. We focussed on a number of items on which we made both progress during the work-in and plans for carrying the work forward after the work-in. Magnesium was of interest, especially MgVII contribution functions. Alessandro and Mike did R-matrix calculations for the excitation and Stuart initiated the configuration average ionisation calculations. We have some results for this already including accurate contributions for MgVI. Martin's *adas409_generate_gtn* is part of this development. Randall and Allan are doing systematic R-matrix calculations (radiation damped) for the he-like and inner shell li-like iso-electronic sequences and a number of ions are complete. Attention was given to assembling the best data for iron ions by Peter, Nigel and Mike. Generalised collisional radiative modelling came up, with special interest in the effects on N/V/OV line ratios and the difference with the simpler astrophysical type of calculation (Gerry, Guilio, Martin and Hugh). The work-in gave some momentum to systematic ionisation calculations and the pursuit of an Ionisation project (equivalent to the DR project) under the direction of Stuart.

3. Forward plans for ADAS release v2.10

Looking forward, for release v2.10, we wish to finally tie up our heavy species and non-Maxwellian developments. By this, I mean essentially the ADAS structural and handling side of these matters. Clearly detailed calculations and data to feed into the structure will carry on for many years to come. We also wish to complete the hardening and usability issues for GCR modelling – time consuming tasks which are largely invisible to the user. Hopefully with these complete and release v2.10 out around the September workshop, we will be able to get on with some new things. At the moment, the ADAS home team see that as bringing the whole special feature area of ADAS properly into play, but we are open to suggestions and it will of course come up again at the workshop.

4. Code and data updates in v2.9.

Corrections and additions to codes (ADAS v2.8 to ADAS v2.9)

C.1 Added the missing *d8tran.pro* routine. The *read_adf35.pro* routine for reading filter files will not work without this. It was inadvertently missed on its release. The *all* argument which returns the data as found in the adf35 dataset has been replaced by *fulldata* to maintain consistency across the read_adf routines

C.2 In ADAS408, particularly when invoked via the IDL *run_adas408.pro* method, IDL could exit before the fortran process had finished writing the output files so causing the files not to be written or be incomplete. This mostly occurred when dealing with filtered output. The fortran code now tells IDL when it is finished.

C.3 An incorrect type of parameter was passed between subroutines in ADAS310. This error did not affect previous results but might have become an issue depending on the compiler/hardware used.

The *run_adas310.pro* IDL version can now write an adf26 bundle-n population file as an output if requested. Two new keywords are also added: */help* to output helpful information and */pbar* which displays a progress bar when running.

C.4 The general progress bar routine did occasionally show negative percentages. Although this did not affect any results it has been corrected.

C.5 There have been many internal changes to and reorganising of ADAS311. The code has now been aligned with the latest developments made by Harvey Anderson before his departure. The dimension of the *gamaf* dependent routines are changed to 500 in order to be consistent with other central ADAS routines. The parameter lists of some routines have also been changed so check these before linking them with your existing personal programs.

Dynamic beam modelling codes need the projection matrix data which can be generated by ADAS311. The hitherto unused second passing file can now be selected to store this data in a format agreed with our IAP/TUW colleagues in Vienna.

With this additional output, there are minor differences in the output panel. More descriptive labels for the passing files are provided, namely, 'adf26 bundle-n populations' and 'projection matrices'. At least one of these outputs must be selected for the code to continue. Note that if both are selected a progress bar showing the population calculation is followed by another for the projection matrix calculation.

C.6 We have now bought the calculation of local Stark/Zeeman emission feature from H (D/T) beams into play as an IDL procedure call *adas305_get_stark* or withing Fortran by calling the *stark.for* routine in the adas3xx library.

The beam, plasma, E and B fields and observation orientation must be specified. General geometry specification is defined by direction cosines. The polarisation can be specified by multipliers on the pi and sigma components.

The feature is returned as either a collection of component wavelengths and emissivities or a Doppler broadened feature over a specified wavelength range (specify minimum and maximum wavelengths and number of pixels).

Note that there is no interactive code yet.

C.7 The adas3xx library has additional routines due to the updating of ADAS311 and the addition of the ADAS305 routines to the central system. Some necessary routine were missed out of the adas2xx library and have now been included. A new adas8xx library has also been added.

C.8 *read_adf12.pro* has been upgraded to remove the restriction that only one parameter could be varied at a time. Also an effective emissivity coefficient is returned if a target temperature (along with donor and receiver masses) is supplied. This removes the need to do the mono-energetic beam/Maxwellian plasma convolution separately. If this temperature is not supplied the returned coefficients are as before.

C.9 ADAS211 and ADAS212 have been upgraded to handle non-Maxwellian modelling. This is work done by Paul Bryans and appears in the interactive input screen as an extra button. When this is pressed, a non-Maxwellian widget pops up on which an analytic or numerical (from file) non-Maxwellian distribution function may be chosen. The rest of the program is transparent to the whether a Maxwellian or non-Maxwellian is chosen. Note that the mean energy of a non-Maxwellian takes the role of temperature for tabulations (see the ADAS manual).

C.10 The following Fotran subroutines required for bound-free and free-free Gaunt factors have been moved to the *fortran/adaslib/*atomic directory.

argam.for
f21.for
fdip0.for
fdip1.for
fdip2.for
fdip.for
fmon1.for

C.11 A collision strength quadrature routine has been added in IDL and Fortran, *h9int.for* and *h9int.pro*. These are needed for subroutine versions of ADAS809 for converting adf04 type 1 files to adf04 type 3 or 4 files. Note that they expect the contents of the adf04 to be read externally. The data structure coming from *read_adf04* is suitable as an input for the IDL version. These developments are necessary to facilitate Monte-Carlo sampling for error assessment in rate coefficients.

C.12 The opacity code, ADAS214, can now be driven by direct IDL call with the *run_adas214.pro* procedure. A potential memory overwrite problem was removed in the fortran code. Note that there are still some problems in running the code in the non-scan mode.

C.13 *run_adas809.pro* has been added as a procedure for direct IDL call. At the same time, we have fixed some things including a badly dimensioned array and the IDL now explicitly waits for the fortran to finish before closing it's I/O pipe.

C.14 We have added the */help* keyword to the IDL procedures *read_adf00.pro, read_adf01.pro, read_adf02.pro, read_adf07.pro, read_adf08.pro, read_adf11.pro, read_adf13.pro, read_adf14.pro, read_adf15.pro, read_adf22.pro, read_adf24.pro* and *read_adf35.pro*.

C.15 Support has been added for 16 bit colour displays - an extension of previous support of 24 bit colour.

C.16 An *xxcomments.pro* IDL procedure has been added which reads the comments from an adf dataset and returns them as an array of strings.

C.17 With some Sun compilers, writing the adf04 files in ADAS801 and ADAS8#1 caused an error because a temporary scratch file was not closed.

C.18 Two new commands are added to help with GCR Project work:

filter04.x : Filters an adf04 file to re-order levels, remove unphysical A-values and to remove levels above the ionisation potential.

merge04.x: Merge two adf04 files - usually an 801 file is supplemented with higher quality data.

Both of these are command line programs and their functionality will be replaced by ADAS705 some time in the future.

C.19 Lorne Horton's *continuo* program has been added as a subroutine both in fortran and IDL form. The new continuo subroutine returns the total continuum emissivity and the free-free only part (in ph cm^3 s^-1 A^-1) for a requested ionisation stage. The original program considered a hydrogen plasma with one impurity in ionisation balance. This functionality can be easily implemented by the user.

C.20 The *xxcase.for* fortran utility routine to convert the case of an input string had the unfortunate property of converting all but the last letter. This has been corrected.

C.21 We have added an *xxdata_09* fortran reading routine along with its IDL counterpart.

C.22 The *run_adas405.pro* IDL procedure can now return a 2D (Te,Ne) fractional abundance and radiated power arrays when the */all* keyword is set.

It is also possible to selectively replace adf11 input files if the input structure "files" is specified. The usual way of using a userid, year and element is still required but these choices can now be superceded on a file by file basis.

run_adas406 has also been updated with these changes.

C.23 We have removed obsolete IDL *loadstate/savestate* statements from ADAS808.

C.24 The non-interactive *run_adas306.pro*, the nlj version of *run_adas308.pro*, is now available. The output is similar to the 308 version but is split by J.

C.25 A new non-interactive IDL procedure, *adas409_generate_gtn.pro*, has been included to facilitate the automatic generation of GTN contribution functions.

Input to the routine is an adf15 photon emissivity coefficient file and adf11 dataset identifiers (year and user id or optional files structure). An adf16 file with an entry for each transition in the adf15 PEC dataset is produced. The recombination contribution is identified and included unless the */norecom* switch is used.

If the adf15 input dataset is metastable resolved the appropriate partitioned adf11 data is used for the ionisation balance and the various metastable PECs are identified.

If temperature and density output grids are not specified the code uses the density grid from the adf15 dataset and a temperature grid of 100 points spanning the region of maximum coronal fractional abundance of the ion. A user defined temperature is also allowed.

The most appropriate temperature range is identified by means of a threshold parameter - a default of 1.0E-3 is used.

A *read_adf16* routine is provided to retrieve and interpolate the contribution function data.

Note that the solar hydrogen abundance is NOT included in the GTN definition unlike our older simpler G(Te) functions of format adf20 which do include it.

C.26 A number of poorly chosen names for common blocks, structures and helper routines in compound widgets were behind the odd behaviour when ADAS310 was run following ADAS312 or ADAS313.

Fortunately just a few programs were affected and the problem was restricted to the interactive performance and not the underlying calculations. The situation has been corrected.

C.27 A new, optional, output file is added to ADAS204 which records the populations of the representative n-shells as b_n and c_n factors. As this is a new addition the old defaults file will not work.

The non-interactive IDL procedure, *run_adas204.pro*, has also been extended to include a population 'popfile' optional output.

Corrections and updates to data (ADAS v2.8 to ADAS v2.9)

D.1 Revised adf09 files have been installed for B-like sequence as follows:

za00#b_mg7ic23.dat
za00#b_mg7ls23.dat
za00#b_na6ic23.dat
za00#b_na6ls23.dat
za00#b_ne5ic23.dat
za00#b_ne5ls23.dat

replacing previous data were incorrect.

D.2 Na-like isoelectronic sequence dielectronic recombination coefficient and associated files of format adf09, adf27 and adf28 files have been added – prepared by Zikri Altun.

D.3 We have renamed some adf09/za00#b files for naming consistency as follows :

za00#b_alic23.dat -> za00#b_al8ic23.dat
za00#b_alls23.dat -> za00#b_al8ls23.dat

D.4 Baseline adf04 data for copper at LS and IC resolutions have been added in a directory adf04/copmm#29. The adf34 driver files can be found in *adf34/copper*.

D.5 adf11 data in the '89' approximation have been added for copper and molybdenum along with the adf03 driver files.

D.6 PEC files for transport analysis of elements which are not yet part of the GCR project are archived in the *adf15/transport* directory and have the template name *transport_llu#<el><iz><ic>.dat*. The 'ic' is optional depending on whether the file is J resolved or not.

A warning message is included in the comments that these files are not part of the GCR project and that there may be significant variability in the data quality between ionisation stages of the same element.

Data for $Cu^{25}+$ and Cu^{26+} have been added in this release.

The adf04 data is taken from the Sampson collection and these have been added to the *adf04/copsm#be* and *adf04/copsm#li* directories.

D.7 Removed files:

adf09/nrbjc00#li/jc00#li_p12ic22.dat
adf09/nrbjc00#li/jc00#li_si11ic22.dat
adf09/nrbjc00#li/jc00#li_xe51icr22.dat
adf09/nrbjc00#li/jc00#li_s13ic22.dat
adf09/nrbjc00#li/jc00#li_ti19ic22.dat

These were previously superceded by nrb versions.

D.8 There is an updated file:

adf09/nrbjc00#li/nrb00#li_zn27icr22.dat

What was meant to be ICR data was infact IC data, but processed with ICR energies (which was why the total differed from IC). The update is by Nigel Badnell

D.9 Further replacements are:

adf09/nrbjc00#be/jc00#be_zn26ic22.dat
adf09/nrbjc00#be/jc00#be_zn26ls22.dat

with:

adf09/nrbjc00#be/nrb00#be_zn26ic22.dat
adf09/nrbjc00#be/nrb00#be_zn26ls22.dat

D.10 Further added files are:

adf09/nrbjc00#be/jc00#be_fe22ic12.dat
adf27/lilike/jc00#li/fe22ic12.dat
adf27/lilike/jc00#li/fe22ic12-2.dat
adf27/lilike/jc00#li/fe22ic12-n.dat
adf27/lilike/jc00#li/fe22ic12_str.dat

which had been computed for the Be-like sequence during the original calculations but had not been archived.

D.11 The adf03 parameter data for carbon had an incorrect upper ion charge which caused ADAS408 to fail. This has been corrected.

D.12 Added Na-like DR sequence, i.e. directories:

adf09/za00#na
adf27/nalike/za00#na
adf28/nalike/za00#na

D.13 Corrections to B-like DR from Nigel Badnell, updates to files:

adf09/za00#b/za00#b_mg7ic23.dat
adf09/za00#b/za00#b_mg7ls23.dat
adf09/za00#b/za00#b_na6ic23.dat
adf09/za00#b/za00#b_na6ls23.dat
adf09/za00#b/za00#b_ne5ic23.dat
adf09/za00#b/za00#b_ne5ls23.dat

D.14 Addition of adf09/adf27/adf28 files for missing odd elements between Ar and Zn (i.e. Co, Cu, K, Mn, Sc and V) for H-like DR.

D.15 Updates to O-like DR (in adas/adf09/oiz00#o)
oiz00#o_al5ls23.dat wasn't even an adf09 file
oiz00#o_al5ic22.dat was calculated with the wrong nuclear charge
oiz00#o_al5ls22.dat was calculated with the wrong nuclear charge

Addition of 2s1 2p5 1P1 parent to oiz00#o_al5ic23.dat
Addition of final levels to oiz00#o_co19ic22.dat and final terms to oiz00#o_co19ls22.dat
Different atomic structure used for oiz00#o_cu21ic23.dat and oiz00#o_cu21ls23.dat, energy levels are now closer to NIST.
Addition of final levels to oiz00#o_cr16ic22.dat and final terms to oiz00#o_cr16ls22.dat
Addition of parents to oiz00#o_si6ic23.dat and oiz00#o_si6ls23.dat
Addition of final levels to oiz00#o_zn22ic23.dat and final terms to oiz00#o_zn22ls23.dat
Addition of 2p6 parent to oiz00#o_fe18ic23.dat

oiz00#o_fe18ic23.dat was calculated with the wrong nuclear charge
oiz00#o_kr28ic23.dat was calculated with the wrong nuclear charge

D.16 Updates to He-like DR
Addition of Cu data (was missing)
Wrong nuclear charge was used for vandium (ic 1-2), corrected.
Wrong nuclear charge was used for magnesium (ic 1-2), corrected.

D.17 Updates to Na-like DR
Added the following files which had previously been sent but were missed (by Allan Whiteford):
adf28/nalike/za00#na/s5icm33.dat
adf28/nalike/za00#na/ca9icm23.dat
adf28/nalike/za00#na/ni17icm23.dat
adf28/nalike/za00#na/ni17ls23.dat
adf28/nalike/za00#na/ti11icm33.dat
adf28/nalike/za00#na/ti11ls33.dat

D.18 Updates to Na-like DR
Added adf09 files to adf09/za00#na for Co, Cu, K, Mn, Sc and V
Added adf27 files to adf27/nalike/za00#na for Co, Cu, K, Mn, Sc and V
Added adf28 files to adf28/nalike/za00#na for Co, Cu, K, Mn, Sc and V

D.19 Addition of adf09/adf27/adf28 files for missing odd elements between Ar and Zn (i.e. Co, Cu, K, Mn, Sc and V) for B-like DR.

D.20 Addition of adf09/adf27/adf28 files for missing odd elements between Ar and Zn (i.e. Co, Cu, K, Mn, Sc and V) for Li-like DR.

D.21 New data for Na-like Zn DR in "ICR" coupling

D.22 Correction to C-like adf09 files:
oiz00#c_ni22ic23.dat had all but the ground parent marked as autoionising oiz00#c_ni22ls23.dat has had a slight correction to the intermediate state atomic structure

D.23 Addition of C-like DR driver files (adf27 and adf28), these were previously missing.

D.24 Addition of missing driver files for 0-like DR.

D.25 Corrections to O-like DR input files:
Relabelling of level in adf28/olike/oiz00#o/al5ic22.dat
Adjustment of NECOR (from 0 to 10) in adf28/olike/oiz00#o/ca12ic22.dat

Wavefunctions in adf27/olike/oiz00#o/s8ic23-n_rad.dat as incorrect
Missing input files added to adf27/olike/oiz00#o/

D.26 Addition of DR data for 1-2 core excitations in the Be-like sequence
Includes adf09, adf27 and adf28 files.

D.27 Upate to Be-like DR:
Added adf09 files to adf09/nrbjc00#be for Co, Cu, K, Mn, Sc and V
Added adf27 files to adf27/belike/jc00#be for Co, Cu, K, Mn, Sc and V
Added adf28 files to adf28/belike/jc00#be for Co, Cu, K, Mn, Sc and V

D.28 Correction to Be-like DR due to dimension inconsistency in codes:
Changes to:

adf09/nrbjc00#be/jc00#be_ar14ic23.dat
adf09/nrbjc00#be/jc00#be_ar14ls23.dat
adf09/nrbjc00#be/jc00#be_ca16ic23.dat
adf09/nrbjc00#be/jc00#be_ca16ls23.dat
adf09/nrbjc00#be/jc00#be_cl13ic23.dat
adf09/nrbjc00#be/jc00#be_cl13ls23.dat
adf09/nrbjc00#be/jc00#be_cr20ic23.dat
adf09/nrbjc00#be/jc00#be_cr20ls23.dat
adf09/nrbjc00#be/jc00#be_fe22ic23.dat
adf09/nrbjc00#be/jc00#be_fe22ls23.dat
adf09/nrbjc00#be/jc00#be_kr32icr23.dat
adf09/nrbjc00#be/jc00#be_mo38icr23.dat
adf09/nrbjc00#be/jc00#be_ni24ic23.dat
adf09/nrbjc00#be/jc00#be_ni24ls23.dat
adf09/nrbjc00#be/jc00#be_o4ic23.dat
adf09/nrbjc00#be/jc00#be_o4ls23.dat
adf09/nrbjc00#be/jc00#be_p11ic23.dat
adf09/nrbjc00#be/jc00#be_p11ls23.dat
adf09/nrbjc00#be/jc00#be_s12ic23.dat
adf09/nrbjc00#be/jc00#be_s12ls23.dat
adf09/nrbjc00#be/jc00#be_si10ic23.dat
adf09/nrbjc00#be/jc00#be_si10ls23.dat
adf09/nrbjc00#be/jc00#be_xe50icr23.dat
adf09/nrbjc00#be/jc00#be_zn26ic23.dat
adf09/nrbjc00#be/jc00#be_zn26icr23.dat
adf09/nrbjc00#be/jc00#be_zn26ls23.dat

D.29 Addition of adf09/adf27/adf28 files for missing odd elements between Ar and Zn (i.e. Co, Cu, K, Mn, Sc and V) for N-like DR.

D.30 Addition of missing adf27 and adf28 input files for F-like DR.

D.31 Addition of missing adf27 and adf28 input files for Ne-like DR.

D.32 Helium type-I error file added (helike_idp04he0_t1.err) corresponding to errors in the associated adf04 file (helike_idp04he0_t1.dat). These uncertainites are estimates based on considerations of each transition and what data exist as well as the quality of the data (in terms of the method and comparison to other datasets).

D.33 Helium type-III error file added, this files contained propagated uncertainties (via Monte Carlo sampling) in the .dat (helike_pb04he0.dat) file, uncertaintes in the collision strengths came from the type-I .err file.

D.34 Changed 0.00E+00 to 1.00E-74 in all of the adf15 files containing 0.00E+00, modified files were:

pec93#c/pec93#c_pjr#c0.dat
pec93#c/pec93#c_pjr#c3.dat

pec93#cr/pec93#cr_llr#cr0.dat
pec93#mo/pec93#mo_llr#mo0.dat
pec96#c/pec96#c_pjr#c0.dat
pec96#c/pec96#c_pjr#c1.dat
pec96#c/pec96#c_pjr#c3.dat
pec96#c/pec96#c_pju#c0.dat
pec96#c/pec96#c_pju#c1.dat
pec96#c/pec96#c_vsr#c1.dat
pec96#c/pec96#c_vsu#c1.dat
pec96#n/pec96#n_pjr#n4.dat
pec96#n/pec96#n_pju#n2.dat
pec96#ne/pec96#ne_pjr#ne1.dat
pec96#ne/pec96#ne_pjr#ne4.dat
pec96#ne/pec96#ne_pjr#ne7.dat
pec96#o/pec96#o_pjr#o0.dat
pec96#o/pec96#o_pjr#o5.dat
pec96#o/pec96#o_pju#o0.dat

D.35 Renamed adf27/helike/mb00#he/*.str files to *_str.dat

D.36 Changes to directory adf28/helike/mb00#he, driver files were duplicated because adasdr only needs one driver file:
The following files were removed:
al11ic23-n.dat
ar16ic23-n.dat
b3ic12-n.dat
b3ic23-n.dat
b3ls12-n.dat
b3ls23-n.dat
be2ic12-n.dat
be2ic23-n.dat
be2ls23-n.dat
c4ic23-n.dat
c4ls23-n.dat
ca18ic23-n.dat
cl15ic23-n.dat
co25ic23-n.dat
cr22ic23-n.dat
f7ic12-n.dat
f7ic23-n.dat
f7ls23-n.dat
fe24ic12-n.dat
fe24ic23-n.dat
fe24ls23-n.dat
k17ic23-n.dat
kr34ic12-n.dat
kr34ic23-n.dat
li1ic12-n.dat
li1ic23-n.dat
li1ls23-n.dat
mg10ic23-n.dat
mn23ic23-n.dat
mo40ic12-n.dat
mo40ic23-n.dat
n5ic12-n.dat
n5ic23-n.dat
n5ls23-n.dat
na9ic23-n.dat
ne8ic12-n.dat

ne8ic23-n.dat
ne8ls23-n.dat
ni26ic23-n.dat
o6ic12-n.dat
o6ic23-n.dat
o6ls23-n.dat
p13ic23-n.dat
s14ic23-n.dat
sc19ic23-n.dat
si12ic23-n.dat
ti20ic23-n.dat
v21ic23-n.dat
xe52ic12-n.dat
xe52ic23-n.dat
zn28ic12-n.dat
zn28ic23-n.dat

because their corresponding files (e.g. zn28ic23-23.dat) were either identical or had observed energies. None of the -n files had energies, but some of the (e.g.) -23 files did. Consequently, the (-23) part of the filename was removed from the following files:

al11ic23-23.dat
ar16ic23-23.dat
b3ic12-2.dat
b3ic23-23.dat
b3ls12-2.dat
b3ls23-23.dat
be2ic12-2.dat
be2ic23-23.dat
be2ls23-23.dat
c4ic12-2.dat
c4ic23-23.dat
c4ls23-23.dat
ca18ic23-23.dat
cl15ic23-23.dat
co25ic23-23.dat
cr22ic23-23.dat
f7ic12-2.dat
f7ic23-23.dat
f7ls23-23.dat
fe24ic12-2.dat
fe24ic23-23.dat
fe24ls23-23.dat
k17ic23-23.dat
kr34ic12-2.dat
kr34ic23-23.dat
li1ic12-2.dat
li1ic23-23.dat
li1ls23-23.dat
mg10ic23-23.dat
mn23ic23-23.dat
mo40ic12-2.dat
mo40ic23-23.dat
n5ic12-2.dat
n5ic23-23.dat
n5ls23-23.dat
na9ic23-23.dat
ne8ic12-2.dat
ne8ic23-23.dat
ne8ls23-23.dat

ni26ic23-23.dat
o6ic12-2.dat
o6ic23-23.dat
o6ls23-23.dat
p13ic23-23.dat
s14ic23-23.dat
sc19ic23-23.dat
si12ic23-23.dat
ti20ic23-23.dat
v21ic23-23.dat
xe52ic12-2.dat
xe52ic23-23.dat
zn28ic12-2.dat
zn28ic23-23.dat

also, there wad duplication in other files but in ths case the –n versions were better because they had the COREX parameter set correctly. The following files were removed:

f7ls12-2.dat
fe24ls12-2.dat
n5ls12-2.dat
ne8ls12-2.dat
o6ls12-2.dat
li1ls12-2.dat
c4ls12-2.dat
be2ls12-2.dat

and the following had their -n extension removed:

f7ls12-n.dat
fe24ls12-n.dat
n5ls12-n.dat
ne8ls12-n.dat
o6ls12-n.dat
li1ls12-n.dat
c4ls12-n.dat
be2ls12-n.dat

finally, the following files didn't have any duplications but they were renamed to remove the unnecessary part of their extension:

al11ls23-23.dat
ar16ls23-23.dat
ca18ls23-23.dat
cl15ls23-23.dat
co25ls23-23.dat
cr22ls23-23.dat
cu27ic23-23.dat
cu27ls23-23.dat
k17ls23-23.dat
mg10ls23-23.dat
mn23ls23-23.dat
na9ls23-23.dat
ni26ls23-23.dat
p13ls23-23.dat
s14ls23-23.dat
sc19ls23-23.dat
si12ls23-23.dat
ti20ls23-23.dat
v21ls23-23.dat

at this point, it is unknown whether the 'good' or 'bad' driver files were used to create the archived adf09 data.

D.37 Partials added to file adf09/nrbjc00#be/nrb00#be_b1ls222.dat, were previously missing although totals and bundled data remain unchanged.

D.38 Correction to DR data for Be-like B. The files jc00#be_b1[ls,ic]12.dat were basically empty and have been replaced by nrb00#be_b1[ls,ic]12.dat. Note that the totals were present in the jc file and are close to the totals now given in the nrb file.

Addition of files b1ic12-2.dat b1ic12-n.dat b1ic12_str.dat to adf27/belike/nrb00#be and files b1ic12.dat b1ls12.dat to adf28/belike/nrb00#be

D.39 Missing partial added to adf09/nrbjc00#li/nrb00#li_be1ls222.dat.

D.40 Update to adf09/mb00#he/mb00#he_mg10ls12.dat, previoulsy the data were calculated with the wrong nuclear charge.

D.41 Update to adf09/mb00#he/mb00#he_v21ls12.dat, previously the data had the wrong final atomic structure.

D.42 Update to adf28/helike/mb00#he/fe24ls12.dat, the previous file had observed energies which were wrong, these have been removed.

D.43 Addition of Li-like DR adf27 driver files in adf27/lilike/jc00#li. Addition of Li-like DR adf28 driver files in adf28/lilike/jc00#li. Driver files for the original DR sequence elements for the 1-2 core excitation were missing.

D.44 Extended C-like adf09 files up to L=6 (i.e. I electrons) for 2-3 core excitation, previously the data only went up to 3. As a result, files adf09/nrboiz00#c/oiz00#c_XXZZ[ic,ls]23.dat have been replaced by files adf09/nrboiz00#c/nrb00#c_XXZZ[ic,ls]23.dat

D.45 Added adf09/nrboiz00#c/nrb00#c_si8ls23.dat (missing from the old oiz files).

D.46 Added adf09/nrboiz00#c/nrb00#c_kr30icr23.dat, adf09/nrboiz00#c/nrb00#c_mo36icr23.dat adf09/nrboiz00#c/nrb00#c_xe48icr23.dat which were not present in the old oiz files.

D.47 Driver files for the above three changes (D44-46) added to adf27/clike/nrb00#c and adf28/clike/nrb00#c.

D.48 adf09 files for C-like Cd removed, they should never have been calculated in the first place. i.e.

adf09/nrboiz00#c/oiz00#c_cd42ic23.dat
adf09/nrboiz00#c/oiz00#c_cd42ls22.dat
adf09/nrboiz00#c/oiz00#c_cd42ls23.dat

are now gone.

D.49 Removed tabs in the data part of datasets in adf04/copha#h/ directory. Outside of comments tabs cause problems in reading and parsing the data.

D.50 Alessandro Lanzafame has added baseline adf04 data for magnesium at LS and IC resolution in adf04/copmm#12. The driver files can be found in adf34/magnesium.

HPS
26 May. 2005