nov18-01

ADAS Bulletin

This is the third of our regular four monthly bug *ADAS code and data error & minor adjustment releases* and is associated with ADAS version 2.5.4. There are only few error corrections as such. Most of the items in the release concern new data and reorganisations to make their naming more consistent. The largest source of new data stems from the collaborative DR Project and is of intermediate coupling *adf09* format. There are also new adf04 files containing high quality R-matrix collision cross-sections for a variety of ions. The efforts of Don Griffin (*dcg*), Nigel Badnell (*nrb*), Connor Ballance (*cpb*) and Dario Mitnik (*dmm*), James Colgan (*jc*), Martin O'Mullane (*mom*) and Harvey Anderson (*ha*) are acknowledged.

I wish to advise that we are working towards a large release of new codes and a new much upgraded edition of the manual for March 2002. A number of the new codes are working successfully under test locally at Strathclyde and at JET. There have been some enquiries over the last year about ADAS capabilities which touch on the new codes. If anyone urgently wishes access to the test codes before main release, please contact us. New codes include satellite line modelling and fitting, hydrogen series and series limit spectral modelling and fitting, non-Maxwellian extensions, adf04-type 1 data and data handling and photoexcitation and ionisation data.

There has been some queries concerning the hydrogen beam emission and helium metastable beam stopping data in ADAS stemming from the work of Harvey Anderson. Since Harvey has now left the University, it will take a while to check fully if these doubts are well based. In the meantime, can **I** advise caution in the their use.

Corrections and additions to codes

- C.1. New utility routines for handling or manipulating the case (upper or lower) in text strings or in files have been added to /.../idl_adas/fortran/adaslib/. These are xxcase.for which changes an input string to entirely upper or lower case, xxfcse.for which changes all the text in an input file to an output file in upper or lower case, xxopcs.for which opens a file in the case of one's choice. The latter is a variant of the conventional ADAS file opening subroutine xxopen.for.
- C.2. A dimensioning error in *read_adf11* has been corrected. This caused an erratic error on different workstations when reading '74' and '85' datasets.
- C.3. A new read_adf14 has been added to read thermal charge exchange coefficients (TCX) into IDL.
- C.4. A new keyword (/directory) has been added to cw_adas_outfile.pro to accommodate the code ADAS808. The latter is an upcoming program which creates composite iso-nuclear adf34 driver files and is part of our attack on very heavy species.
- C.5. The ADAS207 code has been modified to include wavelength limits and a lower emissivity limit. This restricts the number of transitions to be listed according to the above constraints and allows datasets with a large number of transitions to be handled.
- C.6. The ADAS701 code has been re-synchronised to the current version of *autostructure*.
- C.7. The ADAS702 code has been re-synchronised to the current version of adasdr.
- C.8. A problem with exceeded dimensions in the ADAS216 file integrity subroutine *bgtest.for* has been corrected.

Corrections and updates to data

D.1 First data from the DR Project are included in central ADAS. There are new *adf09* files , together with *adf27* and *adf28* drivers, for the hydogen-like, lithium-like, beryllium-like and nitrogen-like iso-electronic sequences. A reorganisation of the *adf27* and *adf28* files into sub-directories given by author name as for *adf09* files is also implemented. The current central ADAS files have been moved as

/../adf27/hlike/* \rightarrow /../adf27/hlike/mom93#h/*

/../adf28/belike/* \rightarrow /../adf28/belike/mom93#h/* etc. for all sequences from hlike to flike. This does introduce a redundant sub-directory and is not precisely compatible with the adf09 archiving, but it does allow us to put the generic driver files into the $\langle seq \rangle$ like directories and to group the

driver files according to the adf09 structure. Thus the adf09 directory structure /../adas/adf09/appears as

dmm00#n	mom93#be	mom93#he	nrb00#h	nrb93#f	nrb93#n
jc00#be	mom93#c	mom93#li	nrb00#b	nrb93#h	nrb93#ne
jc00#li	mom93#f	mom93#n	nrb00#be	nrb93#he	nrb93#o
mom93#b	mom93#h	mom93#0	nrb93#c	nrb93#li	

and the adf27 (adf28 is the same) directory structure /../adas/adf27/ appears as

```
belike clike helike lilike olike
blike flike hlike nlike
```

with an example of the subdirectory structure of one /.../adas/adf27/lilike/ being jc00#li mom93#li

Both here and in D.2 and D.3 following, note the initials of the contributors: ha – Harvey Anderson, dcg – Don Griffin, nrb – Nigel Badnell, dmm – Dario Mitnik, jc – James Colgan, mom – Martin O'Mullane, cpb – Connor Ballance.

D.2 Recent R-matrix work on adf04 file creation has been placed into central ADAS. These files are also archived at Oak Ridge CFADC. The files are as follow:

```
/../adf04/hlike/hlike_ha00#h0ls.dat
   /../adf04/lilike/lilike_dcg00#c3ls.dat
   /../adf04/lilike/lilike_dcg00#o5ls.dat
   /../adf04/mglike/mglike_dcg00#fe14.dat
   /../adf04/mglike/mglike_dcg00#si2.dat
   /../adf04/mglike/mglike dcg00#ti10.dat
   /../adf04/klike/klike_dcg00#fe7.dat
   /../adf04/clike/clike_nrb01#fe20.dat
   /../adf04/blike/blike_nrb01#fe21.dat
   /../adf04/hlike/hlike_cpb01#fe25.dat
   /../adf04/helike/helike_dcg00#mg10.dat
   /../adf04/flike/flike dcg01#ne1.dat
   /../adf04/blike/blike dmm01#ne5.dat
Older files from Don Griffin have been removed, namely
   /../adf04/lilike/lilike_dcg99#c3ls.dat
   /../adf04/lilike/lilike dcg99#o5ls.dat
```

- D.3 There is a mis-named *adf01* file, namely, /../adf01/qcx#he0/qcx#he0_2s_s_kvi#he2.dat becomes /../adf01/qcx#he0/qcx#he0_2s-s_kvi#he2.dat
- D.4 A new *adf04* file for Ar⁺¹⁵ from Connor Ballance, which stems from the RmaX Project and includes the inner shell excitations, is added, namely, /../adf04/lilike/lilike_cpb01#ar15.dat.
- D.5 For completeness, additional adf04 data from the calculations by Sampson, stemming from the eighties are added -namely, /.../copsm#h/copsm#h_kr35.dat and /.../copsm#he/copsm#he_kr34.dat.
- D.6 There were no thermal charge exchange rates (*adf14*) for neutral helium in central ADAS, although they are in the ORNL-6068 book. Singel and double charge exchange rates have been added in a new file /.../adas/adf14/txc#he0/tcx#he0_he.dat.

H. P. Summers 18 Nov. 2001