Atomic Data and Analysis Structure

Appendices

ADAS data formats

The various permanent data sets in ADAS fall into a number of categories with precisely defined organisation and formatting. The specifications of these are called 'ADAS data formats' or ADF's for short. Those relevant to the this manual are as follow:

ADF04	resolved specific ion data collections

ADF04

Provides all required energy level and rate coefficient data for specified low levels of an ion. The data set is complete for a low level population calculation. Specific level selective free electron recombination and charge exchange recombination is included. Formatting conventions and variable storage are given below.

Utilising subroutines :

ADAS201 ADAS205 ADAS206

ADAS208 ADAS214

'JETSHP.STRIP.FORT(SSSUBL)'

'JETSHP.STRIP.FORT(SSSUBJ)'

Formatted files to ADF04 specification :

Database Status Date = October 28, 1997 Data type = specific ion file Data root = */.../adas/adas/adf04/*

Sequence	*Members*	*Library*	*Comments*	*Resolution*	*Quality*
H-like	H,He,Li,Be,B,C,N,O,F,Ne	copha#h	Anderson (n=1,2,3,4,5)	n & nl	best available
He-like	Li,Be,B,C,N,O,F,Ne	copha#he	Anderson (n=1,2,3,4,5)	l	best available
Li-like	Be,C,N,O,Ne,Mg,Al,Si,S,Ar Ca,Ti,Fe,Ni	coppm#li	McWhirter (n=2,3,4,5)	j	best available
Be-like	C,N,O,Ne,Mg,Al,Si,S,Ar, Ca,Ti,Fe,Ni	copjl#be	Lang (n=2,3)	j	best available
C-like	Ca,Fe,Mg,Ne,O,S,Si	clike	Monsignori-Fossi(n=2)	j	assessed
N-like	Ar,Ca,Mg,S,Si	nlike	Landini(n=2)	j	assessed
O-like	Ne,Mg,Al,Si,S,Ar, Ca,Ti,Fe,Ni	olike	Lang/Summers (n=2)	j	best available

Notes:
1. *copha#h* directory has four groups of members (a) prefix '*bn#h*'=> n--shell, high temperature set (b) prefix '*bn#l*'=>n-shell, low temperature set (c) prefix '*hah*'=> nl-shell, high temperature set (d) prefix '*hal*'=>nl-shell, low temperature set.
2. *copha#he* directory members have prefix '*sm#*'=>initial data based on Sampson calculations. Improved data then introduced where available.
3. There are many specific ion files individually assessed for ions of light elements and ions of special fusion interest in the ADAS database. These are in iso-electronic sequence sub-directories with members named by date and originator as */.../adf04/<seq>like/<seq>like_<source><year><el>.dat*

where <seq> is the ioslectronic sequence symbol, <source> is the orginator's initials, <year> a two digit year number and <el> the element symbol.

4. Lang has prepared a detailed document on adf04 files for matching to SOHO/CDS specific needs as detailed by the 'Blue Book'. This is available in the *datastatus* section of ADAS documentation on the web.

Li-like	Be,C,N,O,Ne,Mg,Al,Si,S,Ar	copsm#li	Sampson/Zhang(n=2,3,4,5)	j	medium
	Ca,Ti,Fe,Ni				
Be-like	C,N,O,Ne,Mg,Al,Si,S,Ar	copsm#be	Sampson/Zhang(n=2)	j	medium
	Ca,Ti,Fe,Ni				
B-like	C,N,O,Ne,Mg,Al,Si,S,Ar	copsm#b	Sampson/Zhang(n=2,3)	j	medium
	Ca,Ti,Fe,Ni				
C-like	N,O,Ne,Mg,Al,Si,S,Ar	copsm#c	Sampson/Zhang(n=2,3)	j	medium
	Ca,Ti,Fe,Ni				
F-like	Ne,Mg,Al,Si,S,Ar	copsm#f	Sampson/Zhang(n=2,3)	j	medium
	Ca,Ti,Fe,Ni				
Ne-like	Mg,Al,Si,S,Ar	copsm#ne	Sampson/Zhang(n=3,4)	j	medium
	Ca,Ti,Fe,Ni				
Na-like	Mg,Al,Si,S,Ar	copsm#na	Sampson/Zhang(n=3,4,5)	j	medium
	Ca,Ti,Fe,Ni				
Li-like	Be,C,N,O,Ne,Mg,Al,Si,S,Ar	copss#li	Superst/dipole i.p.(n=2,3,4,5)	j	low
	Ca,Ti,Fe,Ni				
Be-like	C,N,O,Ne,Mg,Al,Si,S,Ar	copss#be	Superst/dipole i.p.(n=2)	j	low
	Ca,Ti,Fe,Ni				
B-like	C,N,O,Ne,Mg,Al,Si,S,Ar	copss#b	Superst/dipole i.p.(n=2,3)	j	low
	Ca,Ti,Fe,Ni				
C-like	N,O,Ne,Mg,Al,Si,S,Ar	copss#c	Superst/dipole i.p.(n=2,3)	j	low
	Ca,Ti,Fe,Ni				
F-like	Ne,Mg,Al,Si,S,Ar	copss#f	Superst/dipole i.p.(n=2,3)	j	low
	Ca,Ti,Fe,Ni				
Ne-like	Mg,Al,Si,S,Ar	copss#ne	Superst/dipole i.p.(n=3,4)	j	low
	Ca,Ti,Fe,Ni				

Na-like	Mg,Al,Si,S,Ar Ca,Ti,Fe,Ni	copss#na	Superst/dipole i.p.(n=3,4,5)	j	low
Be isonuc.	all ions	copmm#4	Cowan/Born(n=2,3)	j & ls	low
C isonuc.	all ions	copmm#6	Cowan/Born(n=2,3)	j & ls	low
N isonuc.	all ions	copmm#7	Cowan/Born(n=2,3)	j & ls	low
O isonuc.	all ions	copmm#8	Cowan/Born(n=2,3)	j & ls	low
Ne isonuc.	all ions	copmm#10	Cowan/Born(n=2,3)	j & ls	low
Mg isonuc.	all ions	copmm#12	Cowan/Born(n=2,3)	j & ls	low
Si isonuc.	all ions	copmm#16	Cowan/Born(n=2,3)	j & ls	low
Cl isonuc.	all ions	copmm#17	Cowan/Born(n=2,3)	j & ls	low
Ar isonuc.	all ions	copmm#18	Cowan/Born(n=2,3)	j & ls	low
Fe isonuc.	all ions	copmm#26	Cowan/Born(n=2,3)	j & ls	low
Ni isonuc.	all ions	copmm#28	Cowan/Born(n=2,3)	j & ls	low
Kr isonuc.	all ions	copmm#36	Cowan/Born(n=2,3)	j & ls	low

Notes:

1. *copss* filess contain dipole collision rate coefficients only. They are often used for supplementation of higher quality data sets which lack dipole allowed transitions between higher levels.
2. *copmm* files contain dipole and non-dipole non-spin change collision rate coefficients only. Exchange collisions are not present.
3. *copmm* & *copss* files are useful for initial survey and radiated power assessment in ADAS series 4 codes.
4. *copss* & *copmm* files are generally created with Eissner configuration notation for automatic initial set up of metastable resolved collisional radiative recombination/ionisation calculation with ADAS series 2 codes.

Data lines : *Format:*

SYM , IZ , IZ0 , IZ1 , BWNO1 , [(PTRM1) , BWNO2 , (PTRM2) .....] , ADFID

until IND = -1

IND , SPEC , IS , IL , IJ , WNO , [(IP1) , IZTA1 , (IP2) , IZTA2 .....]

-1 , (EORB(I),I = 1, 14)

ZEFF , ITYP , (TEA(I), = 1, MAXT)

until INDU = -1 and INDL = -1

until INDU = -1

ICODE, INDU , INDL , AVAL, (GAM(I),I=1,MAXT)

-1

-1 -1

variable identification :

name	*meaning*
SYM	element symbol in form ##+
IZ	charge of the ion
IZ0	nuclear charge
IZ1	ion charge + 1
BWNO1	ionisation potential of lowest level (cm-1) rel. to 1st parent term.
[PTRM1	term of the 1st parent
BWNO2	ionisation potential of lowest level (cm-1) rel. to 2nd parent term.
PTRM2	term of the 2nd parent
...	]
ADFID	ADAS data file type code
IND	index of level
SPEC	configuration specification of level
IS	multiplicity (2*S+1)
IL	total orbital angular momentum quantum number
IJ	(statistical weight of level - 1)/2
WNO	wave number of level relative to the lowest level (cm-1)
[IP1	index of parent accessible by ionisation
IZTA1	shell weighting factor for ionisation to this parent

IP2	index of parent accessible by ionisation
IZTA2	shell weighting factor for ionisation to this parent
....	]
EORB()	orbital energies (Ryd) (optional - compatible only when level configurations are given in Eissner notation)
ZEFF	set equal to IZ1 for normal usage
ITYP	set equal to 3 for normal usage
TEA()	set of electron temperature (Kelvin)
MAXT	number of temperatures (maximum 8)
ICODE	transition data type code: ' ' => electron impact transition 'P' => proton impact transition 'H' => charge exchange recombination 'R' => free electron recombination
INDU	transition: upper energy level index (case ' ' & 'P') receiving level index (case 'H' & 'R')
INDU	transition: lower energy level index (case ' ' & 'P') recombining parent index (case 'H' & 'R')
AVAL	transition: Einstein A-value (sec-1) (case ' ' & 'P') beam energy (ev/amu) (case 'H') --- not used --- (case 'R')
GAM()	transition: gamma (upsilon) (case ' ' & 'P') rate coefft.(cm**3 sec-1) (case 'H') rate coefft.(cm**3 sec-1) (case 'R')

Items in square brackets are only used by program ADAS208. They are ignored by the other processing programs

Table B4c - example.

```
C + 2        6        3       386241.0(2S)
    1 2S2              (1)0( 0.0)            0.0   {1}2.000
    2 2S1 2P1          (3)1( 4.0)        52419.4   {1}1.000
    3 2S1 2P1          (1)1( 1.0)       102352.0   {1}1.000
    4 2P2              (3)1( 4.0)       137477.7   {X}
    5 2P2              (1)2( 2.0)       145876.1   {X}
    6 2P2              (1)0( 0.0)       182519.9   {X}
    7 2S1 3S1          (3)0( 1.0)       238213.0   {1}1.000
    8 2S1 3S1          (1)0( 0.0)       247170.3   {1}1.000
    9 2S1 3P1          (3)1( 4.0)       259717.9   {1}1.000
   10 2S1 3P1          (1)1( 1.0)       258931.3   {1}1.000

                         .        .        .

   40 2S1 5D1          (1)2( 2.0)       346658.3   {1}1.0
   41 2S1 5F1          (3)3(10.0)       347153.8   {1}1.0
   42 2S1 5G1          (3)4(13.0)       346579.4   {1}1.0
   43 2S1 5G1          (1)4( 4.0)       346579.3   {1}1.0
   44 2S1 5F1          (1)3( 3.0)       344955.8   {1}1.0
   -1      26.47    4.37    3.29    1.32    1.15    1.06    0.69    0.62    0.58    0.57    0.42    0.39    0.37    0.36    0.36
  3.0    3       9.00+03 1.80+04 4.50+04 9.00+04 1.80+05 4.50+05 9.00+05 1.80+06
   4   1 2.16-02 1.17-02 1.58-02 2.23-02 2.28-02 1.95-02 1.31-02 8.79-03 6.81-03
   5   1 2.37+03 3.85-01 3.89-01 3.94-01 3.84-01 3.63-01 3.38-01 3.15-01 3.02-01

                .        .        .

43  30 2.67+02 1.10-03 1.21-03 1.49-03 1.84-03 2.30-03 3.03-03 3.65-03 4.31-03
  43  34 2.87+06 1.91+02 2.16+02 2.69+02 3.23+02 3.86+02 4.78+02 5.53+02 6.31+02
  44  43 7.77+04 7.05+02 8.03+02 9.57+02 1.09+03 1.22+03 1.41+03 1.56+03 1.70+03
   7   1 1.00-30 2.67-01 2.28-01 1.55-01 1.06-01 7.12-02 4.20-02 2.80-02 1.60-02
   7   6 1.00-30 5.32-01 4.48-01 2.86-01 1.79-01 1.05-01 5.09-02 2.84-02 1.51-02
   8   7 1.00-30 3.56+00 2.70+00 1.58+00 9.87-01 6.16-01 3.29-01 1.97-01 1.05-01
R  1  +1         1.64-13 1.17-13 7.42-14 5.28-14 3.82-14 2.54-14 1.83-14 1.26-14
R  2  +1         1.13-12 8.31-13 5.34-13 3.55-13 2.21-13 1.13-13 9.22-14 9.22-14
R  3  +1         3.88-13 2.39-13 1.31-13 8.30-14 5.07-14 2.48-14 1.76-14 1.53-14
R  4  +1         1.60-12 7.60-13 2.95-13 1.36-13 5.69-14 1.62-14 6.70-15 3.54-15

                         .        .        .

R 43  +1         2.31-14 3.60-14 2.72-14 1.50-14 8.87-15 4.42-15 2.12-15 8.88-16
R 44  +1         3.63-14 3.95-14 2.71-14 1.55-14 1.09-14 6.42-15 3.24-15 1.42-15
  -1
  -1  -1
C-------------------------------------------------------------------------------
C
C Combined two specific ion files
C
C Target         : JETXPQ.COPMM#BE.DATA(C2#LS#C)
C Supplementary  : JETSHP.BELIKE.DATA(LDH96#C)
C
C Replace SUPPLEMENTARY level into TARGET level
C
C                     1                 1
C                     2                 2
C                     3                 3
```

```
C                   4                4
C                   5                5
C                   6                6
C                   7                7
C                   8                8
C                   9               10
C                  10                9
C                  11               11
C                  12               12
C
C Code : JETXPQ.ATS.FORT(CADF04)
C
C       16:08  20/10/1997
C
C-------------------------------------------------------------------------------
C Update A values of following transitions from supplementary file
C
C      6   1,   8   1,  11   1,  12   1,   5   4,   6   4,   8   4,  11
C     12   4,   7   5,   8   5,  11   5,  12   5,   8   6,  11   6,  12
C     11   7,  12   7,  11   8,  12   8,  12  11,   9   2,  10   2,   9
C     10   3,  10   9,  10   4,   9   5,   9   6,   7   3,  10   7,   8
C      9   8,  11   3,  11  10,  12   2,  12   9
C
C                                                     Martin O'Mullane
C                                                     28-10-97
C-------------------------------------------------------------------------------
C Comments from target file
C---------------------------------------------------------------------------------
C
C     Generated from Cowan Atomic Structure Program
C     M O'Mullane        15:49  20/10/1997
C
C     SCF method used                      : HR
C     Scale factors for Slater Parameters  : 85 99 75 80 65
C     Optically allowed transitions        : yes
C     Optically forbidden transitions M1   : both
C     Optically forbidden transitions E2   : both
C     Born Collision-Strength  - print     :  9
C                              - forbidden :  0 -> 2
C                              - allowed   :  1 -> 1
C                              - included  : 13,all
C     Parity 1    Parity 2    Allowed
C          761         904       1330     initially
C          349         302        599     reduced
C
C---------------------------------------------------------------------------------
C Comments from supplementary file
C-------------------------------------------------------------------------------
C
C  File generated by compression of a J-resolved file
C
C  Program: ADAS209
C
C  Source file: /export/home/adas/adas/adf04/copjl#be/copjl#be_jl#c2j.dat
C
C  Original level indexing:
C     1    2    3    4    5    6    7    8    9   10
C    11   12   13   14   15   16   17   18   19   20
C  Selection Vector:
C     1    2    2    2    3    4    4    4    5    6
```

```
C     7    8    9   10   10   10   11   11   11   12
C
C  Original parent metastables:
C    (1S)
C  Parent bundling vector:
C     0
C
C
C  Producer: adas
C  Date: 05/03/96
C
C-------------------------------------------------------------------------------
C
C  Ionisation potential to (2S) modified to old (JL1990C) value.
C
C  Lorne Horton 13.3.96
C
C-------------------------------------------------------------------------------
C     Note connection to 2p (2P) parent removed following the example
C     of belike_wjd91#be.dat.
C                                          16.03.1996
C-------------------------------------------------------------------------------
C
C   RADIATIVE RECOMBINATION DATA ADDED
C
C   PROCESSED BY ADAS211 ON :
C   /home/mog/adas/adf08/rrc96#li/rrc96#li_c3ls.old
C
C                                                        Martin O'Mullane
C                                                        20-10-97
C-------------------------------------------------------------------------------
C
C     Dielectronic data is post-processed from Badnell files as follows:
C
C      /u/adas/adas/adf09/mom96#li/mom96#li_c3ls12.dat
C      /u/adas/adas/adf09/mom96#li/mom96#li_c3ls22.dat
C      /u/adas/adas/adf09/mom96#li/mom96#li_c3ls23.dat
C
C     The cross-referencing file is as follows:
C
C      /home/mog/adas/adf18/a09_a04/mom96#be/mom96#be_c2ls.dat
C
C     The parent metastable indices are as follows:
C     N.B.:  The dielectronic data from the 2P parent has been manually
C            deleted.
C
C     1.    1S2 2S1             (2)0( 0.5)
C
C     Dielectronic data added to  27 existing rad. recom. level sets
C
C                                                        Martin O'Mullane
C                                                        22-10-97
C-------------------------------------------------------------------------------
```