ADF18: cross-referencing data

Provides cross-referencing data. Formatting conventions and variable storage are given below.

The data class is being extended in the light of the DR Project and GCR Project. Some organisations may be subject to change

Utilising subroutines :

ADAS204 ADAS208 ADAS212 ADAS310 (ADAS804)

Formatted files to ADF18 specification :

Database Status Date = March 17, 2003 Data type =expansion definition files Data root =/.../adas/adas/adf18/

Library	*Sub-library*	*Utilising code*	*Sequences*	*Elements*	*Comments*
a04_a04		(ADAS804)		n,o	merges specific ion files
a09_a04	nrb93#<iso.seq.>	ADAS212	b,be,c,f,he,li,n,ne,o	he,be,b,c,o	Prepares diel. data for specific ion files
	mom96#<iso.seq.>	ADAS212	b,be,c,he,li	he,c	Prepares diel. data for specific ion files
	drm96#<iso.seq.>	ADAS212	b,be,c,f,he,li,n,ne,o	li,n,o,ne	Prepares diel. data for specific ion files
a09_p204	nrb93#<iso.seq.>	ADAS204	b,be,c,f,he,li,n,ne,o	he,be,b,c,o	Prepares diel. data for bundle-nS models
	nrb96#<iso.seq.>	ADAS204	b,be,c,he,li	he,c	Prepares diel. data for bundle-nS models
	drm96#<iso.seq.>	ADAS204	b,be,c,f,he,li,n,o,ne	li,n,o,ne	Prepares diel. data for bundle-nS models
a17_p208	exp93#<iso.seq.>	ADAS208	b,be,c,h,he,li,n,o	he,be,b,c,o	Maps projection data for association with specific ion files
	exp96#<iso.seq.>	ADAS208	h, he, li, be, b, c, n, o,f,ne	he, li,c, n, o, ne	Maps projection data for association with specific ion files
	exp97#<iso.seq.>	ADAS208	h,	h	Maps projection data for association with specific ion files
p310_a17	bndlen_exp#h0.data*	ADAS310		h	driver and map
p311_a17	bndlen_exp#he0.data*	ADAS311		h	driver and map
(data set)*	ADAS310	bndlen_exp#h0.data		h	driver and map
(data set)*	ADAS311	bndlen_exp#he0.data		he	driver and map

Notes: 1. In the a09_a04 library, 'ls#' as a prfefix or 'ls' as a post fix in member names implies LS coupled data mapping.

2. In the a09_p204 library, ‘n’ as a post fix in member names implies n-shell data for bundle-nS mapping.

3. In the a09_p208 library, ‘ls’ as a post fix in member names implies LS coupled mapping.

4. 1996 is now the year number used for the output from the GCR Project.

4. ADAS310 and ADAS311 drivers now moved into appropriate sub-libraries. * denotes data set – not sub-library

a04_a04 data lines : *Format:*

First draft structure only at this time

variable identification :

name *meaning*

Table B18a

```
Combine two adf04 files

Target
------
/u/hps/adas/adf04/cop98#7/copmm#7_ic#n3.dat

Supplement with
------
/u/hps/adas/adf04/cop98#7/copjl#be_ic#n3.dat

78
Supp    Tar
  1     1
  2     2
  3     3
  4     4
  5     5
  6     6
  7     7
  8     8
  9     9
    …
 66    66
 67    67
 68    68
 69    69
 70    70
 71    71
 72    72
 73    73
 74    74
 75    75
 76    76
```

```
77     77
78     78
```

a09_a04 data lines : *Format:*

/SEQINF/
(PTSYMA(K),K=1,NPARNT)
(NPTSPA(K),K=1,NPARNT)
(NSPSYS(K),K=1,NPARNT)
for IPARNT=1,NPARNT
    IPARNT
    (NSPNA(K,IPARNT), K=1,NSPSYS(IPARNT))
    (NLWSTA(K,IPARNT), K=1,NSPSYS(IPARNT))
    (IMAXSTA(K,IPARNT), K=1,NSPSYS(IPARNT))
    (PLWSTA(K,IPARNT), K=1,NSPSYS(IPARNT))
    (FLWSTA(K,IPARNT), K=1,NSPSYS(IPARNT))
repeat
(N(ISHEL),ISHEL=1,NSHEL)
until end of file
    INDA,LVSYMA,LSZDA, LSPA, LSHA, LPTA, (WGHTA(J),J=1,NSHEL)

variable identification :

name	*meaning*
SEQ	
DSNREF	specific ion reference file for expansion
DSNCPM	condensed projection file

NPARNT	number of parent states
NSHEL	number of n-shells involved in expansion
NLEV	number of energy levels in specific ion file
PTSYMA()	parent (term) symmetry
NPTSPA()	parent spin (multiplicity)
NSPSYS()	numbre of spin systems associated with parent
IPARNT	parent counter
NSPNA(,)	spin of recombined system (multiplicity)
NLWSTA(,)	lowest n-shell included for spin system
IMAXSTA(,)	
PLWSTA(,)	phase space occupancy factor for lowest n-shell for spin system
FLWSTA(,)	fractional parentage for ionisation from lowest level of spin system
N()	n-shells included in expansion
INDA	level index with respect to specific ion file for record
LVSYMA	level symmetry (including configuration) for record
LSZDA	SZD file selector for record (if required)
LSPA	spin system (multiplicity) for record
LSHA	active n-shell for record
LPTA	parent index for record
WGHTA()	weighting for n-shell in expansion for record

Table B18b

```
Specific ion input file
-----------------------
"ADASUSER"/adf04/clike/clike_mom97#c0.dat    : specific ion file

Badnell dielectronic files
--------------------------
"ADASCENT"/adf09/nrb93#b/nrb93#b_c1ls22.dat  : 1st. Badnell file
"ADASCENT"/adf09/nrb93#b/nrb93#b_c1ls23.dat  : 2nd. Badnell file
```

```
Output files
------------------------
"ADASUSER"/pass/postllev.pass         : supplemented spec. ion file
"ADASUSER"/pass/postllev.pass1        : dielectronic data for MAINCL codes

Level cross-reference lists for specific ion and badnell files
---------------------------------------------------------------
```

sp.	bd1.	bd2.	bd3.	bd4.	bd5.	bd6.
1	1	0				
2	2	0				
3	4	0				
4	3	0				
5	5	1				
6	6	2				
7	172	0				
8	7	3				
9	8	6				
10	11	9				
11	42	15				
12	171	84				
13	174	0				
14	173	0				
15	9	68				
16	13	96				
17	10	134				
18	12	10				
19	16	0				
20	17	0				
21	15	14				
22	14	135				
23	18	11				
24	19	13				
25	20	4				
26	35	5				
27	59	7				
28	169	8				
29	25	17				
30	29	19				
31	21	18				
32	30	30				
33	34	22				
34	33	20				
35	31	21				
36	32	32				
37	36	31				
38	37	33				
39	38	35				
40	58	12				
41	64	16				
42	98	23				
43	45	36				
44	54	37				
45	39	38				
46	56	39				
47	60	40				
48	61	41				
49	41	44				

```
     50          50          51
     51          40          43
     52          53          53
     53          51          52
     54          52          54
     55           0           0
     56           0           0
     57           0           0
     58           0           0
     59           0           0
     60           0           0
     61           0           0
     62           0           0
     63           0           0
     64           0           0
```

a09_p204 data lines : *Format:*

/SEQINF/

(PTSYMA(K),K=1,NPARNT)

(NPTSPA(K),K=1,NPARNT)

(NSPSYS(K),K=1,NPARNT)

for IPARNT=1,NPARNT

IPARNT

(NSPNA(K,IPARNT), K=1,NSPSYS(IPARNT))

(NLWSTA(K,IPARNT), K=1,NSPSYS(IPARNT))

(IMAXSTA(K,IPARNT), K=1,NSPSYS(IPARNT))

(PLWSTA(K,IPARNT), K=1,NSPSYS(IPARNT))

(FLWSTA(K,IPARNT), K=1,NSPSYS(IPARNT))

repeat

(N(ISHEL),ISHEL=1,NSHEL)

until end of file

INDA,LVSYMA,LSZDA, LSPA, LSHA, LPTA, (WGHTA(J),J=1,NSHEL)

variable identification :

name	*meaning*
SEQ	
DSNREF	specific ion reference file for expansion
DSNCPM	condensed projection file
NPARNT	number of parent states
NSHEL	number of n-shells involved in expansion
NLEV	number of energy levels in specific ion file
PTSYMA()	parent (term) symmetry
NPTSPA()	parent spin (multiplicity)
NSPSYS()	numbre of spin systems associated with parent
IPARNT	parent counter
NSPNA(,)	spin of recombined system (multiplicity)
NLWSTA(,)	lowest n-shell included for spin system
IMAXSTA(,)	
PLWSTA(,)	phase space occupancy factor for lowest n-shell for spin system
FLWSTA(,)	fractional parentage for ionisation from lowest level of spin system
N()	n-shells included in expansion
INDA	level index with respect to specific ion file for record
LVSYMA	level symmetry (including configuration) for record
LSZDA	SZD file selector for record (if required)
LSPA	spin system (multiplicity) for record
LSHA	active n-shell for record
LPTA	parent index for record
WGHTA()	weighting for n-shell in expansion for record

Table B18c

```
ADAS204 driver dataset.
-----------------------
"ADASCENT"/adf25/bns96#c/bns96#c_c0.dat

Dielectronic recombination files.
---------------------------------
"ADASCENT"/adf09/nrb93#b/nrb93#b_c1ls22.dat    : 1st. file of diel. data
"ADASCENT"/adf09/nrb93#b/nrb93#b_c1ls23.dat    : 2nd. file of diel. data

Output file.
------------
"ADASUSER"/pass/adas204.pass     : passing file (not used at present)

Parent cross-reference lists for maincl and Badnell files
---------------------------------------------------------

    mn.        bd1.        bd2.        bd3.        bd4.        bd5.        bd6.
    ---        ----        ----        ----        ----        ----        ----
      1          1           1
      2          2           2
      3          3           3
      4          4           4
      5          5           0

Supplementary LS-breakdown autoionisation data between parent spin pairs
------------------------------------------------------------------------

  (pmni,isysi ; pmnf)           ncut1    A Auger        slope
  -------------------           -----   ---------       -----
     2     2      1                4    1.115d+09
                                   5    3.967d+09
                                   6    1.750d+09
                                   7    1.077d+09
                                   8    8.581d+08
                                   9    8.595d+08
                                  10    7.019d+08
                                  11    6.149d+08
                                  12    6.373d+08
                                  13    5.763d+08
                                  14    5.194d+08
                                  15    3.699d+08
                                  16    3.000d+08
                                  18    1.672d+08
                                  20    1.038d+08
                                  22    6.726d+07
                                  25    3.781d+07       -5.0
```

a17_p208 data lines : *Format:*

/SEQINF/

(PTSYMA(K),K=1,NPARNT)

(NPTSPA(K),K=1,NPARNT)

(NSPSYS(K),K=1,NPARNT)

for IPARNT=1,NPARNT

IPARNT

(NSPNA(K,IPARNT), K=1,NSPSYS(IPARNT))

(NLWSTA(K,IPARNT), K=1,NSPSYS(IPARNT))

(IMAXSTA(K,IPARNT), K=1,NSPSYS(IPARNT))

(PLWSTA(K,IPARNT), K=1,NSPSYS(IPARNT))

(FLWSTA(K,IPARNT), K=1,NSPSYS(IPARNT))

repeat

(N(ISHEL),ISHEL=1,NSHEL)

until end of file

INDA,LVSYMA,LSZDA, LSPA, LSHA, LPTA, (WGHTA(J),J=1,NSHEL)

variable identification :

name	*meaning*
SEQ	
DSNREF	specific ion reference file for expansion
DSNCPM	condensed projection file
NPARNT	number of parent states
NSHEL	number of n-shells involved in expansion
NLEV	number of energy levels in specific ion file
PTSYMA()	parent (term) symmetry
NPTSPA()	parent spin (multiplicity)
NSPSYS()	numbre of spin systems associated with parent
IPARNT	parent counter

NSPNA(,)	spin of recombined system (multiplicity)
NLWSTA(,)	lowest n-shell included for spin system
IMAXSTA(,)	
PLWSTA(,)	phase space occupancy factor for lowest n-shell for spin system
FLWSTA(,)	fractional parentage for ionisation from lowest level of spin system
N()	n-shells included in expansion
INDA	level index with respect to specific ion file for record
LVSYMA	level symmetry (including configuration) for record
LSZDA	SZD file selector for record (if required)
LSPA	spin system (multiplicity) for record
LSHA	active n-shell for record
LPTA	parent index for record
WGHTA()	weighting for n-shell in expansion for record

Table B18d

```
&SEQINF SEQ='B ',
        DSNREF='"ADASUSER"/adf04/blike/blike_mom97#c1.dat',
        DSNCPM='"ADASUSER"/adf17/cbnm96#b/cbnm96#b_c1ls.dat'
        NPARNT=2,
        NSHEL=5,
        NLEV=67,
&END

      PARENT      :(1S)       :(3P)       :           :           :
      SPINPRT     :1          :3          :           :           :
      NSPNSYS     :1          :2          :           :           :

   PARENT =  1
   -----------
      SPINSYS     :2          :           :           :           :
      LOWESTN     :2          :           :           :           :
      IMAX        :2          :           :           :           :
      LOWESTP     :1.0        :           :           :           :
      FRPARNT     :0.25       :           :           :           :

   PARENT =  2
   -----------
      SPINSYS     :2          :4          :           :           :
      LOWESTN     :2          :2          :           :           :
      IMAX        :1          :2          :           :           :
```

```
       LOWESTP     :1.0        :1.0        :           :           :
       FRPARNT     :0.75       :1.0        :           :           :


 RESOLVED NL  <-- BUNDLE-N                N:1     N:2     N:3     N:4     N:5

INDX CODE                SZD SP SH PT   N-SHELL NORMALISED WEIGHTS
---- ----                --- -- -- --   -------------------------
  1* 2S2 2P    (2)1( 2.5)   0  2  2  1  :       : 0.25  :       :       :
  1  2S2 2P    (2)1( 2.5)   0  2  2  2  :       : 0.25  :       :       :
  2* 2S1 2P2   (4)1( 5.5)   0  4  2  2  :       : 1.00  :       :       :
  3  2S1 2P2   (2)2( 4.5)   0  2  2  1  :       : 0.4167:       :       :
  3  2S1 2P2   (2)2( 4.5)   0  2  2  2  :       : 0.4167:       :       :
  4  2S1 2P2   (2)0( 0.5)   0  2  2  1  :       : 0.0833:       :       :
  4  2S1 2P2   (2)0( 0.5)   0  2  2  2  :       : 0.0833:       :       :
  5  2S1 2P2   (2)1( 2.5)   0  2  2  1  :       : 0.25  :       :       :
  5  2S1 2P2   (2)1( 2.5)   0  2  2  2  :       : 0.25  :       :       :
  6  2S2 3S    (2)0( 0.5)   0  2  3  1  :       :       : 0.1111:       :
  7  2S2 3P    (2)1( 2.5)   0  2  3  1  :       :       : 0.3333:       :
  8  2P3       (4)0( 1.5)   0  4  2  0  :       :       :       :       :
  9  2S2 3D    (2)2( 4.5)   0  2  3  1  :       :       : 0.5556:       :
 10  2P3       (2)2( 4.5)   0  2  2  0  :       :       :       :       :
 11  2S2P 3S   (4)1( 5.5)   0  4  3  2  :       :       : 0.1111:       :
 12  2S2 4S    (2)0( 0.5)   0  2  4  1  :       :       :       : 0.0625:
 13  2P3       (2)1( 2.5)   0  2  2  0  :       :       :       :       :
 14  2S2 4P    (2)1( 2.5)   0  2  4  1  :       :       :       : 0.1875:
 15  2S2P 3S   (2)1( 2.5)   0  2  3  2  :       :       : 0.1111:       :
 16  2S2 4D    (2)2( 4.5)   0  2  4  1  :       :       :       : 0.3125:
 17  2S2 4F    (2)3( 6.5)   0  2  4  1  :       :       :       : 0.4375:
 18  2S2P 3P   (4)2( 9.5)   0  4  3  2  :       :       : 0.1852:       :
 19  2S2P 3P   (4)0( 1.5)   0  4  3  2  :       :       : 0.0371:       :
 20  2S2P 3P   (2)1( 2.5)   0  2  3  2  :       :       : 0.1111:       :
 21  2S2 5S    (2)0( 0.5)   0  2  5  1  :       :       :       :       : 0.0400
 22  2S2 5P    (2)1( 2.5)   0  2  5  1  :       :       :       :       : 0.1200
 23  2S2P 3P   (4)1( 5.5)   0  4  3  2  :       :       : 0.1111:       :
 24  2S2 5D    (2)2( 4.5)   0  2  5  1  :       :       :       :       : 0.2000
 25  2S2 5F    (2)3( 6.5)   0  2  5  1  :       :       :       :       : 0.2800
 26  2S2 5G    (2)4( 8.5)   0  2  5  1  :       :       :       :       : 0.3600
 27  2S2P 3P   (2)2( 4.5)   0  2  3  2  :       :       : 0.1852:       :
 28  2S2P 3P   (2)0( 0.5)   0  2  3  2  :       :       : 0.0371:       :
 29  2S2P 3D   (4)3(13.5)   0  4  3  2  :       :       : 0.2592:       :
 30  2S2P 3D   (4)2( 9.5)   0  4  3  2  :       :       : 0.1852:       :
 31  2S2P 3D   (2)2( 4.5)   0  2  3  2  :       :       : 0.1852:       :
 32  2S2P 3D   (4)1( 5.5)   0  4  3  2  :       :       : 0.1111:       :
 33  2S2P 3D   (2)3( 6.5)   0  2  3  2  :       :       : 0.2592:       :
 34  2S2P 3D   (2)1( 2.5)   0  2  3  2  :       :       : 0.1111:       :
 35  2S2P 3S   (2)1( 2.5)   0  2  3  0  :       :       :       :       :
 36  2S2P 3P   (2)2( 4.5)   0  2  3  0  :       :       :       :       :
 37  2S2P 3P   (2)1( 2.5)   0  2  3  0  :       :       :       :       :
 38  2S2P 3P   (2)0( 0.5)   0  2  3  0  :       :       :       :       :
 39  2S2P 3D   (2)2( 4.5)   0  2  3  0  :       :       :       :       :
 40  2S2P 3D   (2)3( 6.5)   0  2  3  0  :       :       :       :       :
 41  2S2P 3D   (2)1( 2.5)   0  2  3  0  :       :       :       :       :
 42  2S2 3S    (4)1( 5.5)   0  4  3  0  :       :       :       :       :
 43  2S2 3P    (2)0( 0.5)   0  2  3  0  :       :       :       :       :
 44  2S2 3S    (2)1( 2.5)   0  2  3  0  :       :       :       :       :
 45  2S2 3P    (4)2( 9.5)   0  4  3  0  :       :       :       :       :
 46  2S2 3P    (4)1( 5.5)   0  4  3  0  :       :       :       :       :
 47  2S2 3P    (2)2( 4.5)   0  2  3  0  :       :       :       :       :
 48  2S2 3S    (2)2( 4.5)   0  2  3  0  :       :       :       :       :
```

```
 49  2S2 3P    (2)1( 2.5)   0  2  3  0  :       :       :       :       :
 50  2S2 3P    (4)0( 1.5)   0  4  3  0  :       :       :       :       :
 51  2S2 3D    (4)3(13.5)   0  4  3  0  :       :       :       :       :
 52  2S2 3D    (2)1( 2.5)   0  2  3  0  :       :       :       :       :
 53  2S2 3D    (4)2( 9.5)   0  4  3  0  :       :       :       :       :
 54  2S2 3P    (2)3( 6.5)   0  2  3  0  :       :       :       :       :
 55  2S2 3D    (4)1( 5.5)   0  4  3  0  :       :       :       :       :
 56  2S2 3D    (2)3( 6.5)   0  2  3  0  :       :       :       :       :
 57  2S2 3D    (2)2( 4.5)   0  2  3  0  :       :       :       :       :
 58  2S2 3P    (2)2( 4.5)   0  2  3  0  :       :       :       :       :
 59  2S2 3P    (2)1( 2.5)   0  2  3  0  :       :       :       :       :
 60  2S2 3D    (2)4( 8.5)   0  2  3  0  :       :       :       :       :
 61  2S2 3D    (2)3( 6.5)   0  2  3  0  :       :       :       :       :
 62  2S2 3D    (2)2( 4.5)   0  2  3  0  :       :       :       :       :
 63  2S2 3D    (2)0( 0.5)   0  2  3  0  :       :       :       :       :
 64  2S2 3D    (2)1( 2.5)   0  2  3  0  :       :       :       :       :
 65  2S2 3S    (2)0( 0.5)   0  2  3  0  :       :       :       :       :
 66  2S2 3P    (2)1( 2.5)   0  2  3  0  :       :       :       :       :
 67  2S2 3D    (2)2( 4.5)   0  2  3  0  :       :       :       :       :
```

a23_a04 data lines : *Format:*

/SEQINF/

(PTSYMA(K),K=1,NPARNT)

(NPTSPA(K),K=1,NPARNT)

(NSPSYS(K),K=1,NPARNT)

for IPARNT=1,NPARNT

IPARNT

(NSPNA(K,IPARNT), K=1,NSPSYS(IPARNT))

(NLWSTA(K,IPARNT), K=1,NSPSYS(IPARNT))

(IMAXSTA(K,IPARNT), K=1,NSPSYS(IPARNT))

(PLWSTA(K,IPARNT), K=1,NSPSYS(IPARNT))

(FLWSTA(K,IPARNT), K=1,NSPSYS(IPARNT))

repeat

(N(ISHEL),ISHEL=1,NSHEL)

until end of file

INDA,LVSYMA,LSZDA, LSPA, LSHA, LPTA, (WGHTA(J),J=1,NSHEL)

variable identification :

name	*meaning*
SEQ	
DSNREF	specific ion reference file for expansion
DSNCPM	condensed projection file
NPARNT	number of parent states
NSHEL	number of n-shells involved in expansion
NLEV	number of energy levels in specific ion file
PTSYMA()	parent (term) symmetry
NPTSPA()	parent spin (multiplicity)
NSPSYS()	numbre of spin systems associated with parent
IPARNT	parent counter
NSPNA(,)	spin of recombined system (multiplicity)
NLWSTA(,)	lowest n-shell included for spin system
IMAXSTA(,)	
PLWSTA(,)	phase space occupancy factor for lowest n-shell for spin system
FLWSTA(,)	fractional parentage for ionisation from lowest level of spin system
N()	n-shells included in expansion
INDA	level index with respect to specific ion file for record
LVSYMA	level symmetry (including configuration) for record
LSZDA	SZD file selector for record (if required)
LSPA	spin system (multiplicity) for record
LSHA	active n-shell for record
LPTA	parent index for record

WGHTA() weighting for n-shell in expansion for record

Table B18c

```
Specific ion input file
------------------------
"ADASCENT"/adf04/belike/belike_jl1990c.dat    : specific ion file for supplementation

Ionisation file (Griffin)
--------------------------
"ADASUSER"/adf23/grf95#be/belike_th_c2ls.dat   : file of ionis. & excit/auto. data

Output files
------------------------
"ADASUSER"/pass/adas213_adf04.pass            : supplemented specific ion file

Term/parent cross-reference lists for specific ion and ionisation file
-------------------------------------------------------------------------
  adf04-trm   adf23-trm
  ---------   ---------
      1           1
      2           2

  adf04-ptrm  adf23-ptrm
  ----------  ----------
     +1          +1
     +2          +2

C-------------------------------------------------------------------------
C
C  Note
C  ----
C  (a) For ionisation, different adf23-lvls referenced to the same adf04-lvl
C      implies summing over the multiple adf23-lvls and accumulating in the
C      adf04-lvl.
C  (b) For excitation, no radiative A-value is entered in the first column
C      following the transition indexing.  This must be added separately if
C      the excitation line is not present in the original data set.  If there
C      is already an excitation transition line, then the radiative A-value is
C      kept and the collisional-data is substituted.
C  (c) '+' signs are used for parent indices.
C  (d) Term coupling datas sets have 'trm' in the headings.  Intermediate
C       coupling datasets have 'lvl' in the headings.
C-------------------------------------------------------------------------
```