ADF23: state selective electron impact ionisation coefficients

Formatting conventions and variable storage suggested for transfer files from Pindzola/Griffin ionisation calculations. Data for an ion is specified by the isoelectronic sequence of the initial (ie. ionising) ion and nuclear charge of the element. An indexed list of LS resolved final (ionised) ion terms is given, with the metastables distinguished by *'s. The other final terms are ordinary terms which may occur as the final term of a direct ionising or autoionising event. An indexed list of terms of the initial ion is given composed of the initial metastable terms (*'d) and then an LS resolved set of auto-ionising terms accessible by excitation. These are relevant to population stucture of the ionising ion. A table of autoionisation rates follows the list connecting the resolved initial ion autoioising terms to the various resolved final terms. There are then distinct blocks of data for each LS-resolved initial metastable term. The direct ionisation rates to the resolved final terms are given first. These data may incorporate autoionisations via parents not identified in the final term list. Then the direct excitations to the resolved autoionising terms are given. Sub-blocks then follow according to spin system and final parent. Only data for the *'d parent metastables is given. A representative n-shell indexing is used. This index is associated to n-shell in an immediately following block which gives the autoionisation rates to the metastable parent terms. Excitation to parent and spin system separated autoionising n-shells is then given. Representative bundle-n levels are used. In this organisation, ionisation and excitation data is provided as a function of temperature. Up to 10 temperatures may be given with some preference for using the temperature set Te(k)=z1**2*theta(k)

where z1 is the recombining ion charge and theta = 1.0d3, 2.0d3, 5.0d3,1.0d4, 2.0d4,5.0d4, 1.0d5, 2.0d5, 5.0d5, 1.0d6

Utilising subroutines :

JETSHP.ADAS9120.fort(ADAS204)-generalised collisional dielectronic calculations

JETSHP.ADAS9120.fort(ADAS208)-low level population/projection calculation, line emission and power

Formatted files to ADF23 specification :

Database Status Date = July, 29 1996 Data type =cio files Data root =/.../adas/adas/adf23/

Ionising seq.	*Members*	*Library*	*Prefix*	*Comments*	*Quality*
H-like.		grf95#h	th	LS resolution	medium
He-like	b3,be2,c4,n5,o6	grf95#he	th	LS resolution	medium
Li-like	b2,be1,c3,n4,o5	grf95#he	th, exp	LS resolution	medium
Be-like	b1,be0,c2,n3,o4	grf95#he	th	LS resolution	medium
B-like	b0,c1,n2,o3	grf95#he	th	LS resolution	medium
C-like	c0,n1,o2	grf95#he	th, exp	LS resolution	medium
N-like	n0,o1	grf95#he	th, exp	LS resolution	medium
N-like	o0	grf95#he	th, exp	LS resolution	medium

Notes: 1. The prefixes ‘th’ indicates that the normalisation of the state selective metastable resolved data is to give consistency with the best available theoretical data for the unresoved inisation from the ground state. The prefixes ‘exp’ indicates that the normalisation of the state selective metastable resolved data is to give consistency with the best available experimental data for the unresoved inisation from the ground state.

Data lines : *Format:*

seq='SEQ' nucchg=IZ0 ADFID

final term indexing bwnf= BWNF nprf = NPRF

---

indf code S L WJ wnf

---- ---- - - -- ----------

for indf=1,NPRF

INDF CCFI TRFI WNFI

repeat

initial term indexing bwni= BWNI nlev = NLEV

---

indf code S L WJ wnf

---- ---- - - -- ----------

for indi=1,NLEV

INDI CCII TRII WNII

repeat

Auger rates

---

indi\indf 1 2 3 .... NPRF

---

for indi=(.ne.*), NLEV

```
          INDI            AA1IF     AA2IF     AA3IF  .... NPRF
repeat
for INDI=1,NLEV(.and.*)
          ------------------------------------------
          meti*=MI  nsys = NSYSI  nrep=NREP

          ionis rates
          -----------
              indf  Te=     TE1       TE2       TE3      TE4       TE5       TE6  .....
               ----  ---
          for indf=1,NPRF
                        INDF       QI1IF     QI2IF     QI3IF     QI4IF     QI5IF     QI6IF                    repeat
          excit rates
           -----------
              indi  Te=     TE1       TE2       TE3      TE4       TE5       TE6  .....
              ----  ---
          for indi=1,NLEV (indi.ne.*)
                        INDI       EX1II     EX2II     EX3II     EX4II     EX5II     EX6II  .                repeat
          for metf=1,NPRF (metf.eq.*)
                    for isys=1,NSYS
                                                          --------------------------
                                                          metf*=MF sys =IS spnsys=SS
                              Auger rates
                              -----------
                              irep   n    f =       IF1       IF2  ....
```

---- - -

for irep=1,NREP

IREP N AN1IF AN2IF T6I

repeat

excit rates

----

irep Te= TE1 TE2 TE3 TE4 TE5 TE6 . ---- ---

for irep=1,NREP

IREP N1II EN2II EN3II EN4II EN5II EN6II repeat

repeat

repeat

repeat

variable identification :

name	*meaning*
SEQ	sequence identifier for initial ion (two characters)
IZ0	nuclear charge
ADFID	ADAS data file type code (ADF23)
BWNF	binding wave number of lowest final term (cm-1)
NPRF	number of final terms
INDF	ndex of final terms
CCFI	configuration (or Eissner code thereof) for final term
TRFI	term and weight (wt=2*wj+1) specification for term
WNFI	energy of final term relative to lowest (cm-1)
BWNI	binding wave number of lowest initial term (cm-1)

NLEV	number of terms specified in initial ion
INDI	index of initial terms
CCII	configuration (or Eissner code thereof) for initial term
TRII	term and weight (wt=2*wj+1) specification for term
WNRI	energy of initial term relative to lowest (cm-1)
AA1IF,--	Auger rates from initial (autoionising only) terms to final terms (sec-1)
MI	initial ion metastable index
NSYSI	number of spin systems for autoionising n-shells of initial ion
NREP	number of representative n-shells of initial ion
TE1 ,--	electron temperatures (K)
QI1IF,--	ionisation rate coefficients from initial metastable term to final terms (cm+3 sec-1)
EX1II,--	excitation rate coefficients from initial metastable term to autoionising initial ion terms (cm+3 sec-1)
MF	final ion metastable index
IS	initial ion spin system index
SS	initial ion spin (2S+1)
IF1 ,--	index of final metastable terms
IREP	index of representative n-shells
N	principal quantum number
AN1IF,--	Auger rate coefficients (sec-1) from nS shell of initial ion to final metastable term
EN1II,--	Excitation rate coefficients to nS shell built on

final parent metastable MF from initial metastable MI

Table B23c - example.

```
seq ='Cl'    nucch1 =18                                                    ADF23

  final term indexing        bwnf =    328458.6     nprf = 23
  --------------------
  indf    code           S L   WJ       wnf
  ----    ----           - -   --  ------------
    1  3s23p43d0        (3)1( 4.0)          0.0
    2  3s23p43d0        (1)2( 2.0)      13662.9
    3  3s23p43d0        (1)0( 0.0)      32915.2
    4  3s13p53d0        (3)1( 4.0)     113957.2
    5  3s13p53d0        (1)1( 1.0)     143670.4
    6  3s23p33d1        (5)2(12.0)     144347.9
    7  3s23p33d1        (3)2( 7.0)     156397.7
    8  3s23p33d1        (1)2( 2.0)     177069.5
    9  3s23p33d1        (1)0( 0.0)     182642.8
   10  3s23p33d1        (3)3(10.0)     185207.6
   11  3s23p33d1        (3)3(10.0)     186062.5
   12  3s23p33d1        (3)2( 7.0)     187014.3
   13  3s23p33d1        (3)1( 4.0)     187417.5
   14  3s23p33d1        (3)4(13.0)     190272.7
   15  3s23p33d1        (1)4( 4.0)     195257.2
   16  3s23p33d1        (1)1( 1.0)     202572.6
   17  3s23p33d1        (3)0( 1.0)     204177.6
   18  3s23p33d1        (3)2( 7.0)     210194.4
   19  3s23p33d1        (3)1( 4.0)     213598.1
   20  3s23p33d1        (1)3( 3.0)     213799.7
   21  3s23p33d1        (1)1( 1.0)     251893.0
   22  3s23p33d1        (1)2( 2.0)     252207.5
   23  3s23p33d1        (1)3( 3.0)     253118.9

  initial term indexing      bwni =    222905.6     nlev =  3
  --------------------
  indi    code           S L   WJ       wni
  ----    ----           - -   --  ------------
    1  3s23p53d0        (2)1( 2.5)          0.0
    2  3s23p43d1        (4)2( 9.5)     131991.6
    3  3s23p43d1        (4)3(13.5)     142702.5

-------------------------------------------------------------------------------
meti*= 1

  ionis rates
  -----------
  indf Te= 8.00D+03  2.00D+04  4.00D+04  8.00D+04  2.00D+05  4.00D+05  8.00D+05  2.00D+06  4.00D+06  8.00D+06  2.00D+07  4.00D+07
  ---- ---
    1      1.05D-26  1.13D-15  6.32D-12  5.18D-10  7.46D-09  1.85D-08  2.93D-08  3.75D-08  3.83D-08  3.57D-08  2.96D-08  2.45D-08
    2      4.51D-28  2.26D-16  2.12D-12  2.26D-10  3.83D-09  9.99D-09  1.63D-08  2.13D-08  2.20D-08  2.06D-08  1.72D-08  1.42D-08
    3      2.45D-30  1.08D-17  2.07D-13  3.21D-11  6.82D-10  1.92D-09  3.26D-09  4.38D-09  4.58D-09  4.33D-09  3.64D-09  3.03D-09
    4      4.35D-36  5.59D-20  1.45D-14  8.11D-12  4.07D-10  1.59D-09  3.16D-09  4.54D-09  4.73D-09  4.38D-09  3.53D-09  2.85D-09
    5      6.54D-39  2.18D-21  1.66D-15  1.60D-12  1.12D-10  4.89D-10  1.04D-09  1.55D-09  1.65D-09  1.55D-09  1.26D-09  1.02D-09
    6      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
    7      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
    8      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
    9      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
   10      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
   11      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
```

12	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
13	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
14	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
15	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
16	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
17	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
18	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
19	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
20	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
21	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
22	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
23	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00

---

meti*= 2

ionis rates

indf	Te= 8.00D+03	2.00D+04	4.00D+04	8.00D+04	2.00D+05	4.00D+05	8.00D+05	2.00D+06	4.00D+06	8.00D+06	2.00D+07	4.00D+07
1	3.22D-15	8.71D-11	2.87D-09	1.73D-08	5.20D-08	7.34D-08	8.29D-08	7.99D-08	7.11D-08	6.03D-08	4.62D-08	3.68D-08
2	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
3	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
4	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
5	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
6	9.42D-28	1.80D-16	1.16D-12	1.02D-10	1.65D-09	4.33D-09	6.96D-09	8.63D-09	8.44D-09	7.50D-09	5.82D-09	4.59D-09
7	7.06D-30	5.05D-18	5.05D-14	5.53D-12	1.02D-10	2.82D-10	4.65D-10	5.88D-10	5.80D-10	5.18D-10	4.04D-10	3.20D-10
8	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
9	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
10	2.12D-31	3.55D-18	1.01D-13	1.88D-11	4.80D-10	1.48D-09	2.60D-09	3.44D-09	3.47D-09	3.14D-09	2.48D-09	1.97D-09
11	3.63D-31	6.68D-18	1.97D-13	3.70D-11	9.55D-10	2.95D-09	5.20D-09	6.89D-09	6.95D-09	6.29D-09	4.97D-09	3.95D-09
12	2.73D-32	5.57D-19	1.70D-14	3.25D-12	8.48D-11	2.63D-10	4.65D-10	6.16D-10	6.21D-10	5.63D-10	4.45D-10	3.53D-10
13	1.37D-31	2.92D-18	9.03D-14	1.74D-11	4.57D-10	1.42D-09	2.51D-09	3.33D-09	3.36D-09	3.04D-09	2.40D-09	1.91D-09
14	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
15	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
16	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
17	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
18	2.84D-33	7.32D-19	5.19D-14	1.52D-11	5.13D-10	1.74D-09	3.23D-09	4.44D-09	4.55D-09	4.17D-09	3.32D-09	2.65D-09
19	3.93D-34	1.47D-19	1.18D-14	3.68D-12	1.29D-10	4.44D-10	8.30D-10	1.15D-09	1.18D-09	1.08D-09	8.61D-10	6.88D-10
20	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
21	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
22	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
23	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00

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meti*= 3

ionis rates

indf	Te= 8.00D+03	2.00D+04	4.00D+04	8.00D+04	2.00D+05	4.00D+05	8.00D+05	2.00D+06	4.00D+06	8.00D+06	2.00D+07	4.00D+07
1	2.21D-14	1.85D-10	4.09D-09	2.02D-08	5.32D-08	7.14D-08	7.83D-08	7.39D-08	6.51D-08	5.48D-08	4.17D-08	3.31D-08
2	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
3	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
4	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
5	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
6	6.57D-27	3.90D-16	1.70D-12	1.23D-10	1.76D-09	4.42D-09	6.94D-09	8.45D-09	8.21D-09	7.25D-09	5.61D-09	4.41D-09
7	4.92D-29	1.09D-17	7.38D-14	6.65D-12	1.09D-10	2.88D-10	4.64D-10	5.77D-10	5.65D-10	5.02D-10	3.90D-10	3.08D-10
8	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00
9	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00

```
   10      2.12D-30  1.10D-17  2.12D-13  3.23D-11  7.33D-10  2.17D-09  3.72D-09  4.84D-09  4.84D-09  4.36D-09  3.43D-09  2.72D-09
   11      9.06D-31  5.16D-18  1.03D-13  1.59D-11  3.64D-10  1.08D-09  1.86D-09  2.42D-09  2.42D-09  2.18D-09  1.72D-09  1.36D-09
   12      7.62D-31  4.82D-18  9.94D-14  1.57D-11  3.62D-10  1.08D-09  1.86D-09  2.43D-09  2.43D-09  2.19D-09  1.72D-09  1.37D-09
   13      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
   14      1.63D-30  1.47D-17  3.41D-13  5.71D-11  1.37D-09  4.13D-09  7.17D-09  9.41D-09  9.44D-09  8.52D-09  6.71D-09  5.33D-09
   15      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
   16      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
   17      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
   18      1.62D-33  1.29D-19  6.21D-15  1.50D-12  4.48D-11  1.46D-10  2.65D-10  3.58D-10  3.64D-10  3.32D-10  2.63D-10  2.10D-10
   19      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
   20      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
   21      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
   22      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
   23      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
C-------------------------------------------------------------------------
C  Data generated by Donald C. Griffin   on 08/17/96
C
C  The rates involving ionization from the  3p subshell of the ground-state
C  configuration were determined using the experimental data of:
C  Mueller et al.
C  The rates for all other subshells were generated from configuration-
C  average cross sections, with non-relativistic wavefunctions , using the
C  relaxed-core approximation, the post form  for the scattering potentials,
C  and the  natural-phase approximation.
C  They were then multiplied by the appropriate angular coefficients.
C-------------------------------------------------------------------------
```