ADF06: resolved specific ion data collections for ion impact

Provides energy level and rate coefficient data for specified low levels of an ion. The data set contains processes driven by ion impact. The data is intended to supplement other codes and is not complete, or suitable, for a stand-alone population calculation. Specific level selective ionisation may be included. Formatting conventions and variable storage are given below.

Utilising subroutines :

ADAS208 adas7#3

Formatted files to ADF06 specification :

Database Status	Date = March 17, 2003	Data type = specific ion file	Data root = */.../adas/adas/adf04/*		
Sequence	*Members*	*Library*	*Comments*	*Resolution*	*Quality*

Data lines : *Format:*

SYM , IZ , IZ0 , IZ1 , STRG1	1a3,i2,2i10,1a75
until IND = -1	
IND , CFG, IS , IL , C8, STRG2	i5,1x,1a18,1x,i1,1x,i1,1a8,1a56
-1 ,	i5
ZEFF , ITYP , STRG4	f5.1,i5,6x,1a112
until INDU = -1 and INDL = -1	
until INDU = -1	
MT, ZP, MP, PROJSTR	‘/mt=’,fm.n,’/zp=’,fm.n, ’/mp=’,fm.n,’/’,a,’/’
CCODE, INDU , INDL , STRG5	1a1,1i3,i4,1a128
-1	
-1 -1	

variable identification :

name	*meaning*		
SYM	element symbol in form ##+		
IZ	charge of the ion		
IZ0	nuclear charge		
IZ1	ion charge + 1		
STRG1	*fword1(cword1)fword2(cword2)*…where the *fword* are fixed point decimal numbers and *cword* are character strings		
	[*fword1* = BWNO =BWNOA(1)	ionisation potential (cm-1)	fm.n
	fwordi = BWNOA(I)	ionisation potential (cm-1) of lowest level relative to the ith parent	fm.n
	cwordi=MLTP,LP	$(2S_p+1)L_p$ for ith parent in LS coupling	1i1,1a1
	cwordi=MLTP,LP,XJ	$(2S_p+1)L_p\ J_p$ for ith parent in IC coupling	1i1,1a1,fm.n
	If *cword1* is missing, the parent ground state is assumed to be ^{1}S. If further *fword*s are present they must be paired with *cword*s. In LS coupling the parent weight is $(2S_p+1)(2L_p+1)$. In IC coupling the parent weight is $(2J_p+1)$. The number of parents is denoted byy NPRT.]		
IND	index of level		
CFG	configuration specification of level. The specification is at the user's choice. Adoption of Eissner or Standard configuration forms are required for automatic operation of advanced codes. [Eissner form for CFG is *cword=cshell1cshell2cshell3……*where *cshelli=50+q,indi* *q* is the number of equivalent electrons in the ith shell and *indi* is the shell index in the Eissner collating sequence: 1=1s, 2=2s, 3=2p, 4=3s,…,9=4d, 0=4f, A=5s,…,E=5g,…, Z=8j, a=9s,… For the 1st shell, *50+q* may be replaced by *q* without error. Standard form for CFG is *cword1 cword2 cword3 …* where *cwordi=nlq* *n* is the principal quantum number collating sequence: 1=1, 2=2, 9=9, a=10,b=11, l is the orbital angular momemum quantum number character s,p,d,… q is the equivalent electron collating sequence: 1=1, , 9=9, a=10,b=11.		

	Note that *cwordi* is always of format 1a3.]		
IS	multiplicity (2*S+1)		
IL	total orbital angular momentum quantum number		
C6	*(XJ)*		1a1,f3.1,1a1
		or	1a1,f4.1,1a1
	where *XJ*= (statistical weight of level - 1)/2 in LS coupling and *XJ*=J in IC coupling		
STRG2	*fword{cword1}fword1{cword2}fword2*…where *fword, fwordi* are fixed point decimal numbers and *cwordi* are characters		
	fword = WNO	excitation energy (cm-1) relative to lowest level	fm.n
	[*cwordi*=IPRT	parent index with reference to list on first line	
	'X'	if ionisation from this level is an excluded process	1a1
	fwordi = ZTA	fractional parentage factor for ionisation to ith parent	fm.n]
ZEFF	effective ion charge set equal to IZ1 for normal usage		
ITYP	=1 => ion impact collisional data given as omegas as a function of X parameter		
	=2 => no longer in use		
	=3 => ion impact collisional data given as Upsilons as a function of T_e (the usual form)		
	=4 => reserved for non-Maxwellian rate coefficients		
STRG4	fword1 fword2 …	where the fword are floating point numbers omitting the 'e' or 'd'	14e8.2
	fwordi = XA(I) ith value of threshold parameter for ITYP=1		
	fwordi = TEA(I) ith value of electron temperature (K) for ITYP=3		
	Note that a maximum number of temperatures MAXT=14 is allowed with ITYP=3. 50 values of threshold parameter are allowed with ITYP=1.		
CCODE	transition data type code as follows: ' ' => unspecified electron impact excitation data '1' => dipole electron impact excitation data '2' => non-dipole, non-spin change electron impact excitation data '3' => spin change electron impact excitation data 'i' or 'I' =>electron impact ionisation data from stage below 's' or 'S' =>electron impact ionisation data to stage above		

MT	Mass of target (IZ0) in atomic mass units	
ZP	Charge of projectile	
MP	Mass of projectile in atomic mass units	
PROJSTR	<mass>^<symbol>, eg 2^He for fully stripped He as the projectile	
INDU	transition: upper energy level index (case ' ', '1', '2', '3')	
	receiving level index (case 'I')	
	ionising level index (case 'S')	
INDL	transition: lower energy level index (case ' ', '1', '2', '3'')	
	ionised parent index (case 'S') – should be preceded by a '+'	
	ionising daughter index (case 'I') – should be preceded by a '-'	
STRG5	fworda fword1 … fwordn fwordb where the fword are floating point numbers	
	omitting the 'e' or 'd'	16e8.2 (16e8.2)
	fworda = AVAL transition: Einstein A-value for E2 only (sec-1) (case ' ', '1', '2', '3')	
	otherwise blank	
	fwordi = OMGI Omega for ith energy (ITYP=1, case ' ', '1', '2', '3')	
	= GAMI Upsilon for ith temperature (ITYP=3, case ' ', '1', '2', '3' & 'P')	
	= SIONI scaled ionisation rate coefft. $M^{3/2}\exp(I_{ion}/kT_e)$ S (cm**3 sec-1) for ith temperature with I_{ion} , the level ionisation energy and S the ionisation rate coefficient (case'S', 'I')	
	[fwordb = BETL Bethe high energy limit value (ITYP=3, case ' ', '1', '2')	
	otherwise not present.]	

Table B6c – example of the basic file structure.

```
 FE+22        26        23  15732424.0413
    1 522               (1)0( 0.0)              0.0000
    2 512513            (3)1( 0.0)           351556.5227
    3 512513            (3)1( 1.0)           383269.1320
    4 512513            (3)1( 2.0)           473412.2740
    5 512513            (1)1( 1.0)           762599.0790
    6 523               (3)1( 0.0)           964386.4116
    7 523               (3)1( 1.0)          1033038.9872
    8 523               (3)1( 2.0)          1081279.7275
   -1
23.00    3       5.29+04 1.06+05 2.64+05 5.29+05 1.06+06 2.64+06 5.29+06 1.06+07 2.64+07 5.29+07 1.06+08 2.64+08 5.29+08 1.06+09
/mt = 5.58470e1 /zp = 1.00e0 /mp = 1.00794e0 /  1^H  impact /
   7   1 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00
   8   1 2.42+03 3.34-88 3.13-57 3.41-31 5.32-19 3.45-11 3.46-05 1.50-02 7.81-01 2.05+01 9.95+01 2.89+02 6.89+02 1.02+03 1.29+03 1.58+03
   3   2 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00
   4   2 6.76-01 1.36-35 1.25-21 1.23-10 2.21-05 6.24-02 3.80+01 6.60+02 3.61+03 1.15+04 1.77+04 2.20+04 2.49+04 2.59+04 2.63+04 2.64+04
   5   2 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00
   4   3 3.29-01 7.07-31 1.39-18 9.93-09 4.54-04 5.20-01 1.55+02 2.02+03 9.47+03 2.73+04 4.02+04 4.90+04 5.48+04 5.67+04 5.75+04 5.79+04
   5   3 4.66+01 2.91-58 4.96-37 2.11-19 2.42-11 6.33-06 1.37-01 9.96+00 1.27+02 7.89+02 1.66+03 2.55+03 3.37+03 3.70+03 3.86+03 3.85+03
   5   4 4.48+00 1.26-52 2.01-33 1.23-17 2.61-10 1.93-05 1.57-01 7.77+00 7.70+01 3.86+02 7.26+02 1.03+03 1.27+03 1.36+03 1.40+03 1.39+03
   7   6 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00
   8   6 6.18-01 6.72-35 3.48-21 2.34-10 3.44-05 8.54-02 4.66+01 7.70+02 4.11+03 1.30+04 2.00+04 2.48+04 2.82+04 2.92+04 2.97+04 2.99+04
   8   7 1.08-02 2.79-23 5.55-14 3.33-06 1.41-02 3.41+00 3.05+02 2.50+03 9.25+03 2.29+04 3.18+04 3.75+04 4.13+04 4.26+04 4.32+04 4.37+04
/mt = 5.58470e1 /zp = 1.00e0 /mp = 2.00000e0 /  2^H  impact /
   7   1 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00
   8   1 2.42+03 0.00+00 7.85-66 4.71-36 1.13-21 4.55-13 2.09-06 2.33-03 2.60-01 1.49+01 1.13+02 4.65+02 1.56+03 2.77+03 3.99+03 6.01+03
   3   2 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00
   4   2 6.76-01 8.20-41 1.08-24 4.25-12 4.46-06 4.04-02 5.91+01 1.41+03 9.30+03 3.54+04 5.96+04 7.87+04 9.30+04 9.78+04 9.99+04 1.00+05
   5   2 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00
   4   3 3.29-01 1.94-35 3.97-21 6.15-10 1.35-04 4.34-01 2.78+02 4.74+03 2.60+04 8.69+04 1.38+05 1.77+05 2.05+05 2.14+05 2.18+05 2.20+05
   5   3 4.66+01 7.52-67 2.05-42 4.76-22 6.90-13 1.12-06 9.05-02 1.11+01 2.01+02 1.75+03 4.44+03 7.77+03 1.16+04 1.34+04 1.44+04 1.46+04
   5   4 4.48+00 3.02-60 3.43-38 6.36-20 1.28-11 4.93-06 1.38-01 1.10+01 1.49+02 9.84+02 2.14+03 3.37+03 4.55+03 5.06+03 5.30+03 5.30+03
   7   6 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00
   8   6 6.18-01 4.95-40 3.64-24 8.79-12 7.37-06 5.74-02 7.35+01 1.64+03 1.05+04 3.97+04 6.68+04 8.84+04 1.05+05 1.10+05 1.13+05 1.14+05
   8   7 1.08-02 1.38-26 7.51-16 5.71-07 8.23-03 4.40+00 7.07+02 7.00+03 2.86+04 7.78+04 1.14+05 1.38+05 1.55+05 1.61+05 1.64+05 1.66+05
/mt = 5.58470e1 /zp = 1.00e0 /mp = 3.00000e0 /  3^H  impact /
   7   1 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00
   8   1 2.42+03 0.00+00 1.93-71 4.24-39 1.03-23 1.86-14 2.32-07 5.03-04 9.65-02 9.57+00 9.99+01 5.27+02 2.25+03 4.57+03 7.29+03 1.31+04
   3   2 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00
   4   2 6.76-01 3.39-44 8.30-27 4.35-13 1.41-06 2.72-02 6.92+01 2.01+03 1.50+04 6.44+04 1.16+05 1.61+05 1.97+05 2.11+05 2.17+05 2.18+05
   5   2 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00
   4   3 3.29-01 2.22-38 7.33-23 9.08-11 5.51-05 3.44-01 3.58+02 7.20+03 4.37+04 1.62+05 2.74+05 3.66+05 4.37+05 4.62+05 4.74+05 4.79+05
   5   3 4.66+01 1.89-72 6.05-46 7.31-24 6.30-14 3.20-07 5.79-02 9.87+00 2.28+02 2.51+03 7.27+03 1.41+04 2.29+04 2.77+04 3.06+04 3.18+04
```

```
   5   4 4.48+00 3.20-65 2.60-41 1.88-21 1.63-12 1.81-06 1.09-01 1.17+01 1.94+02 1.56+03 3.79+03 6.44+03 9.32+03 1.07+04 1.14+04 1.15+04
   7   6 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00 0.00+00
   8   6 6.18-01 2.37-43 3.18-26 9.49-13 2.42-06 3.95-02 8.69+01 2.35+03 1.69+04 7.17+04 1.30+05 1.80+05 2.22+05 2.38+05 2.45+05 2.47+05
   8   7 1.08-02 7.44-29 4.39-17 1.63-07 5.17-03 4.62+00 1.08+03 1.20+04 5.24+04 1.53+05 2.32+05 2.91+05 3.33+05 3.49+05 3.56+05 3.62+05
  -1
  -1  -1


c-------------------------------------------------------------------------------
c  Autostructure / a2iratbf production of adf06 datasets
c
c
c  Script  : /home/mbluteau/svn_adas/adas_dev/adas1#2/branch/mbluteau/scripts/
c            process_ion_irat_adf27_to_adf06.pl
c
c  Codes   : /home/adas/offline_adas/adas7#1/bin/as24.x
c            /home/mbluteau/svn_adas/adas_dev/adas1#2/branch/mbluteau/bin/a2iratbt.x
c  Driver  : /home/mbluteau/svn_adas/adas_dev/adas1#2/branch/mbluteau/adas/adf27/irat/belike/copmmb#be/fe22.dat
c  Outputs : /home/mbluteau/svn_adas/adas_dev/adas1#2/branch/mbluteau/adas/adf06/copmmb#be/ic#fe22.dat.
c
c  Producer: mbluteau
c  Date    : 13-9-2016
c
c-------------------------------------------------------------------------------
```