ADF04: resolved specific ion data collections

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, ionisation and charge exchange recombination are included. Formatting conventions and variable storage are given below. Note that current preferred data for important elements are grouped into isonuclear libraries of the form 'adas#'.

Utilising subroutines :

ADAS201 ADAS205 ADAS206 ADAS208 ADAS214 ADAS215 ADAS407

ADAS705 ADAS706 ADAS809 ADAS810

Formatted files to ADF04 specification :

Database Status Date = March 17, 2003 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	high quality
He-like	Li,Be,B,C,N,O,F,Ne	copha#he	Anderson (n=1,2,3,4,5)	l	high quality
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	high quality
Be-like	C,N,O,Ne,Mg,Al,Si,S,Ar, Ca,Ti,Fe,Ni	copjl#be	Lang (n=2,3)	j	high quality
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.

24 Oct. 1999 revision includes new /lilike/lilike_dcg99#c3ls.dat, /lilike/lilike_dcg99#o5ls.dat and /clike/clike_kma99#o2ic.dat datasets and an update to /helike/helike_kvi97#he0.dat.

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 Ca,Ti,Fe,Ni	copsm#li	Sampson/Zhang(n=2,3,4,5)	j	medium
Be-like	C,N,O,Ne,Mg,Al,Si,S,Ar Ca,Ti,Fe,Ni	copsm#be	Sampson/Zhang(n=2)	j	medium
B-like	C,N,O,Ne,Mg,Al,Si,S,Ar Ca,Ti,Fe,Ni	copsm#b	Sampson/Zhang(n=2,3)	j	medium
C-like	N,O,Ne,Mg,Al,Si,S,Ar Ca,Ti,Fe,Ni	copsm#c	Sampson/Zhang(n=2,3)	j	medium
F-like	Ne,Mg,Al,Si,S,Ar Ca,Ti,Fe,Ni	copsm#f	Sampson/Zhang(n=2,3)	j	medium
Ne-like	Mg,Al,Si,S,Ar Ca,Ti,Fe,Ni	copsm#ne	Sampson/Zhang(n=3,4)	j	medium
Na-like	Mg,Al,Si,S,Ar Ca,Ti,Fe,Ni	copsm#na	Sampson/Zhang(n=3,4,5)	j	medium
Li-like	Be,C,N,O,Ne,Mg,Al,Si,S,Ar Ca,Ti,Fe,Ni	copss#li	Superst/dipole i.p.(n=2,3,4,5)	j	low
Be-like	C,N,O,Ne,Mg,Al,Si,S,Ar Ca,Ti,Fe,Ni	copss#be	Superst/dipole i.p.(n=2)	j	low
B-like	C,N,O,Ne,Mg,Al,Si,S,Ar Ca,Ti,Fe,Ni	copss#b	Superst/dipole i.p.(n=2,3)	j	low
C-like	N,O,Ne,Mg,Al,Si,S,Ar Ca,Ti,Fe,Ni	copss#c	Superst/dipole i.p.(n=2,3)	j	low
F-like	Ne,Mg,Al,Si,S,Ar Ca,Ti,Fe,Ni	copss#f	Superst/dipole i.p.(n=2,3)	j	low
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	copss#na	Superst/dipole i.p.(n=3,4,5)	j	low
	Ca,Ti,Fe,Ni				
H isonuc.	all ions	adas#1	O'Mullane	ls & n	preferred
He isonuc.	all ions	adas#2	O'Mullane	ic & ls	preferred
Li isonuc.	all ions	adas#3	Ballance	ls, bndle-n	preferred
C isonuc.	all ions	adas#6	O'Mullane	ic & ls	preferred
N isonuc.	all ions	adas#7	Dux	ic & ls	preferred
O isonuc.	all ions	adas#8	Broooks	ic & ls	preferred
Ne isonuc.	all ions	adas#10	O'Mullane	ic & ls	preferred
Ar isonuc.	Ar+18 only	adas#18	Whiteford	ic	preferred
H isonuc.	all ions	copmm#1	Cowan/Born(n=1-5)	j & ls	low
He isonuc.	all ions	copmm#2	Cowan/Born(n=1-5)	j & ls	low
Li isonuc.	all ions	copmm#3	Cowan/Born(n=2,3)	ls	low
Be isonuc.	all ions	copmm#4	Cowan/Born(n=2,3)	j & ls	low
B isonuc.	all ions	copmm#5	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
F isonuc.	all ions	copmm#9	Cowan/Born(n=2,3)	j & ls	low
Ne isonuc.	all ions	copmm#10	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
Xe isonuc.	all ions	copmm#54	Cowan/Born(n=2,3)	j & ls	low

Notes: 1. *adas* sub-libraries contain the currently preferred data for the ions of the element. The prefix 'ls' indicates the LS-coupled data complete with all recombination contributions for full generalised collisional-radiative population calculations. The prefix 'ic' indicates intermediate

j-resolved data with spectroscopic quality energies. The latter data sets do not have the recombination contributions. The prefix 'n' indicates n-shell bundled data and is relevant only to the hydorgen-like stage. When a change of preferred data is made, the formerly preferred data is moved back into isoelectronic data collections with an advisory note as to when they were the preferred data.

24 Oct. 1999 revision includes new datasets in /adas#7 and /adas#8 from the GCR project and updates to /adas#2 and /adas#6.

2. *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.
3. *copmm* files contain dipole and non-dipole non-spin change collision rate coefficients only. Exchange collisions are not present.
4. *copmm* & *copss* files are useful for initial survey and radiated power assessment in ADAS series 4 codes.
5. *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 , STRG1	1a3,i2,2i10,1a75
until IND = -1	
IND , CFG, IS , IL , C8, STRG2	i5,1x,1a18,1x,i1,1x,i1,1a8,1a56
-1 , STRG3	i5, 1a95
ZEFF , ITYP , STRG4	f5.1,i5,6x,1a112
until INDU = -1 and INDL = -1	
until INDU = -1	
CCODE, INDU , INDL , STRG5	1a1,1i3,i4,1a128
-1	
-1 -1	
C+++ERROR specification start++++++	1a35
C	
C TCLASS1	1a2,1a
C	
C IL-IU ERROR	1a2,1a,'-',1a, '-',fm.n
C	

C TCLASS2	1a2,1a
C	
C IL-IU ERROR	1a2,1a,'-',1a, '-',fm.n
C	
C+++ERROR specification end++++++++	1a35

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]
[STRG3	*fword1 fword2 fword3*…where *fwordi* are space separated fixed point decimal numbers		
	fwordi = ORB	energy (Ryd) of ith orbital.	fm.n

These are mandatory only for ADAS407 but if present must follow the Eissner collating sequence and commence with 1s.]

ZEFF	effective ion charge set equal to IZ1 for normal usage	
ITYP	=1 => electron collisional data given as omegas as a function of X parameter	
	=2 => no longer in use	
	=3 => electron 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	
	'p' or 'P' => positive ion impact excitation data	
	'r' or 'R' => free electron recombination/capture data	
	'h' or 'H' => charge exchange recombination data from neutral hydrogen	
	'i' or 'I' =>electron impact ionisation data from stage below	
	's' or 'S' =>electron impact ionisation data to stage above	
	'l' or 'L' =>unresolved dielectronic satellite line emission data	
INDU	transition: upper energy level index (case ' ', '1', '2', '3', & 'P')	
	receiving level index (case 'H', 'R', 'L', 'I')	
	ionising level index (case 'S')	
INDL	transition: lower energy level index (case ' ', '1', '2', '3" & 'P')	

recombining parent index (case ‘H’, ‘R’, ‘L’) – should be preceded by a ‘+’

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 (sec-1) (case ‘ ’, ‘1’, ‘2’, ‘3’)

= EBEAM beam energy (ev/amu) (case 'H')

= WVLN unresolved satellite line wavelength (A) (case 'L')

= AAUG Auger rate (sec-1) for doubly excited states (case ‘R’)

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’)

= RCHEXI charge exchange recombinaton rate coefft.(cm**3 sec-1) for the ith temperature (case ‘H’')

= RCOEFI free electron recombinaton rate coefft. (cm**3 sec-1) for the ith temperature (case ‘R’) . Note that this combines radiative and dielectronic recombination unless doubly excited states are directly included in the file. In the latter case the DR resonance capture only is given for the doubly excited state (together with the Auger rate – AAUG above). The stablised singly excited state’s ‘R’ line must then only include radiative recombination to avoid double counting. ‘L’ lines provide any missing unresolved DR to the level in this case

= SIONI scaled ionisation rate coefft. 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.]

The error block is optional and is placed in the comment section at the end of the data set. It is signalled by the start and end line 'ERROR specification' lines.

[TCLASS	Transition class, 'ionisation', excitation','recombination'
IL	lower level of transition. '*' indicates all levels
IU	upper level of transition. '*' indicates all levels.
ERROR	percentage error (uncertainty) in transition data
	Note that sets of transition may be specified as for example '1-*' or '*-*'. Error blocks are analysed by the code ADASA215.]

Items in square brackets are only used by advanced population codes. They are ignored by the simpler processing programs – see the ADAS manual program descriptions for details.

Table B4c – example of the basic file structure.

```
H+ 0         1         1        109679.
   1   1S              (2)0( 0.5)               0.
   2   2S              (2)0( 0.5)           82303.
   3   2P              (2)1( 2.5)           82303.
 .       .       .
  14   5F              (2)3( 6.5)          105348.
  15   5G              (2)4( 8.5)          105348.
  -1
1.00    3       5.80+03 1.16+04 3.48+04 5.80+04 1.16+05 1.74+05 2.32+05 2.90+05
  2   1 0.00+00 2.60-01 2.96-01 3.26-01 3.39-01 3.73-01 4.06-01 4.36-01 4.61-01
  3   1 6.27+08 4.29-01 5.29-01 8.53-01 1.15+00 1.81+00 2.35+00 2.81+00 3.20+00
  4   1 0.00+00 6.51-02 6.96-02 7.76-02 8.13-02 8.70-02 9.21-02 9.66-02 1.01-01
  5   1 1.67+08 1.12-01 1.26-01 1.86-01 2.43-01 3.54-01 4.38-01 5.07-01 5.66-01
 .       .
 12  10 0.00+00 3.48+01 4.05+01 3.97+01 3.70+01 3.32+01 3.11+01 2.98+01 2.89+01
 13  10 5.05+04 7.51+01 1.03+02 1.32+02 1.32+02 1.26+02 1.22+02 1.22+02 1.22+02
 14  10 0.00+00 1.67+02 2.71+02 5.28+02 6.50+02 7.64+02 8.01+02 8.15+02 8.21+02
 15  10 4.26+06 3.87+02 7.33+02 1.76+03 2.46+03 3.64+03 4.48+03 5.14+03 5.69+03
 -1
```

```
C-----------------------------------------------------------------------------
C
C 14/10/99
C _1NEW1ADF04 FILE CREATED FROM THE 39 STATE (RMPS) R-MATRIX CALCULATION
C
C   H. ANDERSON, C. P. BALLANCE, N. R. BADNELL AND H. P. SUMMERS
C                J.PHYS.B33, 1255 (2000)
C
C 31/01/02
C  UPSILONS RECOMPUTED FROM ORIGINAL OMEGA FILE, BUT WITH IMPROVED
C  ASYMPTOTICS. PREVIOUS WERE INCREASINGLY INACCURATE AT .GE. 15EV.
C  NEW RESULTS DIFFER BY .LE. 10% AT .LE. 10EV. FOR DETAILS SEE
C   H. ANDERSON, C. P. BALLANCE, N. R. BADNELL AND H. P. SUMMERS
C                J.PHYS.B35, XXXX (2002)  -  CORRECTION.
C
C 22/04/02
C  Parent term (1S) on line 1 and Bethe limit points on transition lines
C  removed from archived file to show simplest adf04 pattern
C
C-----------------------------------------------------------------------------
```

Table B4d – example of the advanced file structure.

```
C + 3         6         4        520178.4(1S)   2931440.0(3S)
    1 1S2 2S1           (2)0( 0.5)        0.0   {1}1.000 {2}1.500
    2 1S2 2P1           (2)1( 2.5)    64555.4   {1}1.000
    3 1S2 3S1           (2)0( 0.5)   302849.0   {1}1.000
    4 1S2 3P1           (2)1( 2.5)   320071.2   {1}1.000
    5 1S2 3D1           (2)2( 4.5)   324886.1   {1}1.000
    6 1S2 4S1           (2)0( 0.5)   401348.1   {1}1.000
    7 1S2 4P1           (2)1( 2.5)   408319.8   {1}1.000
    8 1S2 4D1           (2)2( 4.5)   410338.5   {1}1.000
    9 1S2 4F1           (2)3( 6.5)   410434.2   {1}1.000
   10 1S2 5S1           (2)0( 0.5)   445368.5   {1}1.000
   11 1S2 5P1           (2)1( 2.5)   448860.5   {1}1.000
   12 1S2 5D1           (2)2( 4.5)   449889.2   {1}1.000
   13 1S2 5F1           (2)3( 6.5)   449939.8   {1}1.000
   14 1S2 5G1           (2)4( 8.5)   449948.4   {1}1.000
   -1      28.35    4.77    4.18    1.99    1.83    1.79    1.08    1.02    1.00    1.00    0.68    0.65    0.64    0.64    0.64
  4.0    3       8.00+03 1.60+04 3.20+04 8.00+04 1.60+05 3.20+05 8.00+05 1.60+06 3.20+06 8.00+06 1.60+07
   3   1 1.00-30 5.68-01 5.49-01 5.16-01 4.46-01 3.96-01 3.84-01 3.87-01 3.83-01 3.83-01 3.85-01 3.86-01
   5   1 4.57+05 4.90-01 4.97-01 5.11-01 5.43-01 5.79-01 6.24-01 7.90-01 9.58-01 1.08+00 1.18+00 1.21+00
  .      .       .
  12  11 5.65+04 1.61+03 1.81+03 2.03+03 2.36+03 2.62+03 2.89+03 3.26+03 3.54+03 3.82+03 4.19+03 4.47+03
```

```
  14   9 1.09+09 1.59+02 1.64+02 1.74+02 2.06+02 2.53+02 3.22+02 4.48+02 5.63+02 6.89+02 8.69+02 1.01+03
   9   1 1.00-30 9.51-02 9.39-02 9.15-02 8.57-02 7.94-02 7.31-02 6.89-02 6.82-02 6.81-02 6.80-02 6.80-02
R  1  +1         4.33-13 3.08-13 2.19-13 1.41-13 1.01-13 7.39-14 9.62-14 1.34-13 1.09-13 4.80-14 2.13-14
R  2  +1         1.41-12 9.87-13 6.84-13 4.08-13 2.67-13 1.66-13 1.34-13 1.66-13 1.33-13 5.71-14 2.43-14
R 12  12 1.65+02 3.42+03 3.64+03 3.96+03 4.98+03 4.70+03 5.02+03 5.45+03 5.77+03 6.09+03 6.51+03 6.83+03
R  3  +1         1.23-13 8.77-14 6.27-14 4.07-14 2.95-14 2.13-14 1.39-14 1.04-14 6.99-15 3.34-15 1.68-15
  .     .
R 13  +2         4.57-10 1.86-10 7.46-11 2.03-11 7.36-12 2.63-12 6.72-13 2.38-13 8.43-14 2.13-14 7.54-15
R 14  +2         9.73-12 3.92-12 1.56-12 4.24-13 1.53-13 5.49-14 1.40-14 4.96-15 1.76-15 4.44-16 1.57-16
H  3  +1         1.00-13 1.42-13 2.00-13 3.67-13 3.40-12 6.46-11 1.02-09 3.98-09 1.11-08 3.02-08 5.13-08
H  4  +1         5.50-12 2.47-11 1.41-10 9.53-10 3.16-09 8.82-09 2.15-08 3.45-08 4.91-08 6.01-08 6.13-08
H  5  +1         1.38-09 1.78-09 2.12-09 2.32-09 2.20-09 1.89-09 1.88-09 4.35-09 1.15-08 2.62-08 3.94-08
H  6  +1         2.12-17 3.00-17 4.25-17 8.52-17 4.76-16 6.14-15 2.00-13 2.74-12 3.10-11 3.01-10 9.08-10
H  7  +1         1.09-16 1.54-16 2.18-16 4.38-16 2.44-15 3.16-14 1.03-12 1.41-11 1.52-10 1.08-09 2.24-09
H  8  +1         3.22-17 4.56-17 6.45-17 1.29-16 7.23-16 9.33-15 3.01-13 4.14-12 5.26-11 8.12-10 3.18-09
H  9  +1         3.72-17 5.26-17 7.46-17 1.49-16 8.35-16 1.08-14 3.51-13 4.80-12 5.46-11 5.37-10 1.78-09
S  1  +1         6.19-10 6.73-10 9.77-10 1.44-09 1.87-09 2.31-09 2.80-09 3.00-09 3.03-09 2.79-09 2.46-09
S  1  +2         4.07-11 4.01-11 3.98-11 5.45-11 8.12-11 1.12-10 1.69-10 2.23-10 2.80-10 3.39-10 3.58-10
 -1
 -1  -1
C-------------------------------------------------------------------------------
C
C Combined two specific ion files
C
C Target         : JETXPQ.COPMM#LI.DATA(C3#LS#B)
C Supplementary  : JETSHP.LILIKE.DATA(CFM96#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               9
C
C
C Code : JETXPQ.ATS.FORT(CADF04)
C
C        14:07  22/10/1997
C
C-------------------------------------------------------------------------------
C
C   Update A values of following transitions from Cowan data
C
C      5   1,   8   1,   4   2,   7   2,   9   2
C
C                                                  Martin O'Mullane
C                                                  27-10-97
C-------------------------------------------------------------------------------
C Comments from target file
C-------------------------------------------------------------------------------
C
C     Generated from Cowan Atomic Structure Program
C
C     M O'Mullane        13:53  22/10/1997
C
```

```
C
C     SCF method used                      : HR
C
C     Scale factors for Slater Parameters  : 75 96 75 75  0
C
C     Optically allowed transitions        : yes
C
C     Optically forbidden transitions M1   : both
C
C     Optically forbidden transitions E2   : both
C
C     Born Collision-Strength  - print     :  9
C
C                              - forbidden :  0 -> 2
C
C                              - allowed   :  1 -> 1
C
C                              - included  : 11,all
C
C     Parity 1    Parity 2    Allowed
C          102         104        161     initially
C           45          30         62     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/coppm#li/coppm#li_pm#c3j.dat
C
C  Original level indexing:
C     1    2    3    4    5    6    7    8    9   10
C    11   12   13   14   15
C  Selection Vector:
C     1    2    2    3    4    4    5    5    6    7
C     7    8    8    9    9
C
C  Original parent metastables:
C    (1S)
C  Parent bundling vector:
C     0
C
C
C  Producer: horton
C  Date: 03/06/96
C
C-------------------------------------------------------------------------------
C
C  Modified to include triplet parent for ionisation
C
C  Costanza F. Maggi  04/06/96
C
C-------------------------------------------------------------------------------
C
C  Energy levels replaced by NIST values.
C
```

```
C                                                       22-10-97
C-----------------------------------------------------------------------------
C
C   RADIATIVE RECOMBINATION DATA ADDED                  Martin O'Mullane
C
C   PROCESSED BY ADAS211 ON :
C   /home/mog/adas/adf08/rrc96#he/rrc96#he_c4ls.dat
C
C                                                       Martin O'Mullane
C                                                       22-10-97
C-----------------------------------------------------------------------------
C
C     Dielectronic data is post-processed from Badnell files as follows:
C
C      /u/adas/adas/adf09/mom96#he/mom96#he_c4ls12.dat
C      /u/adas/adas/adf09/mom96#he/mom96#he_c4ls22.dat
C
C     The cross-referencing file is as follows:
C
C      /home/mog/adas/adf18/a09_a04/mom96#li/mom96#li_c3ls.dat
C
C     The parent metastable indices are as follows:
C
C     1.    1S2                (1)0( 0.0)
C     2.    1S1 2S1            (3)0( 1.0)
C
C     Dielectronic data added to  15 existing rad. recom. level sets
C
C                                                       Martin O'Mullane
C                                                       22-10-97
C-----------------------------------------------------------------------------
C   Thermal charge exchange coefficient lines added for reactions:
C
C   DONOR      RECEIVER   FINAL STATE  SOURCE
C   ---------  ---------  -----------  ----------------------------------
C   H + 0 (1)  C + 4 (1)  3s (2S)      /u/cfm/adas/adf24/scx#h0/scx#h0_cfm#c4.dat
C   H + 0 (1)  C + 4 (1)  3p (2P)      /u/cfm/adas/adf24/scx#h0/scx#h0_cfm#c4.dat
C   H + 0 (1)  C + 4 (1)  3d (2D)      /u/cfm/adas/adf24/scx#h0/scx#h0_cfm#c4.dat
C   H + 0 (1)  C + 4 (1)  4s (2S)      /u/cfm/adas/adf24/scx#h0/scx#h0_cfm#c4.dat
C   H + 0 (1)  C + 4 (1)  4p (2P)      /u/cfm/adas/adf24/scx#h0/scx#h0_cfm#c4.dat
C   H + 0 (1)  C + 4 (1)  4d (2D)      /u/cfm/adas/adf24/scx#h0/scx#h0_cfm#c4.dat
C   H + 0 (1)  C + 4 (1)  4f (2F)      /u/cfm/adas/adf24/scx#h0/scx#h0_cfm#c4.dat
C
C
C
C   Processing code: ADAS509/ADAS505
C   Producer:        C.F. Maggi
C   Date:            16/12/97
C
C-----------------------------------------------------------------------------C
C   Ionisation data added from /u/adas/adas/adf07/szd93#c/szd93#c_c.dat
C
C   Producer : Martin O'Mullane
C   Date     : 23/09/99
C
C-----------------------------------------------------------------------------

C-----------------------------------------------------------------------------
C ADAS ADF04 DATA - SCCS info: @(#)mom97_ls#c3.dat   2.1 Date 01/09/01
```

```
C-------------------------------------------------------------------------------
```

Table B4e – example of a file with an error block set in the comments section. Note that the error block is signalled by 'C+++ERROR specification start++++++' and terminated by 'C+++ERROR specification end++++++++'.

```
HE+ 0         2         1    198310.7722
    1 1s2               (1)0( 0.0)         0.0000
    2 1s2s              (3)0( 1.0)    159856.0776
    3 1s2s              (1)0( 0.0)    166277.5420
    4 1s2p              (3)1( 4.0)    169087.0135
    5 1s2p              (1)1( 1.0)    171135.0000
    6 1s3s              (3)0( 1.0)    183236.8920
    7 1s3s              (1)0( 0.0)    184864.9320
    8 1s3p              (3)1( 4.0)    185564.7049
    9 1s3d              (3)2( 7.0)    186101.6597
   10 1s3d              (1)2( 2.0)    186105.0698
   11 1s3p              (1)1( 1.0)    186209.4684
   12 1s4s              (3)0( 1.0)    190298.2165
   13 1s4s              (1)0( 0.0)    190940.3300
   14 1s4p              (3)1( 4.0)    191217.1603
   15 1s4d              (3)2( 7.0)    191444.5885
   16 1s4d              (1)2( 2.0)    191446.5590
   17 1s4f              (3)3(10.0)    191451.9838
   18 1s4f              (1)3( 3.0)    191452.0005
   19 1s4p              (1)1( 1.0)    191492.8160
   -1
 1.00    3       1.16+05 2.32+05 5.80+05 1.16+06 2.32+06 5.80+06 1.16+07 2.32+07 5.80+07 1.16+08 2.32+08 5.80+08 1.16+09 2.32+09
   2   1 1.00-30 5.25-02 4.14-02 2.96-02 2.01-02 1.26-02 6.25-03 3.47-03 1.85-03 7.83-04 4.00-04 2.03-04 8.19-05 4.11-05 2.05-05
   3   1 1.00-30 5.45-02 6.44-02 8.31-02 1.01-01 1.20-01 1.45-01 1.60-01 1.71-01 1.80-01 1.83-01 1.86-01 1.87-01 1.87-01 1.88-01
  .     .
  18  17 1.00-30 2.18-01 1.10-01 4.43-02 2.22-02 1.11-02 4.45-03 2.23-03 1.11-03 4.45-04 2.23-04 1.11-04 4.46-05 2.23-05 1.11-05
  19  17 1.00-30 7.65-01 4.16-01 1.77-01 9.11-02 4.63-02 1.87-02 9.40-03 4.71-03 1.89-03 9.44-04 4.72-04 1.89-04 9.45-05 4.72-05
  19  18 1.00-30 1.90+02 2.00+02 2.05+02 2.05+02 2.04+02 2.02+02 2.01+02 2.01+02 2.00+02 2.00+02 2.00+02 2.00+02 2.00+02 2.00+02
S  1  +1 1.00-30 8.87-09 1.35-08 2.11-08 2.56-08 2.75-08 2.59-08 2.29-08 1.92-08 1.45-08 1.11-08 7.95-09 5.16-09 4.07-09 3.32-09
  .     .       .
S  2  +1 1.00-30 1.06-07 1.02-07 8.89-08 7.72-08 6.60-08 5.27-08 4.35-08 3.37-08 2.08-08 1.53-08 1.28-08 1.06-08 8.81-09 6.98-09
S 18  +1 1.00-30 1.39-06 1.09-06 7.54-07 5.57-07 4.09-07 2.64-07 1.85-07 1.33-07 9.03-08 6.81-08 5.08-08 3.41-08 2.52-08 1.88-08
S 19  +1 1.00-30 9.16-07 8.10-07 6.59-07 5.50-07 4.49-07 3.06-07 2.13-07 1.60-07 1.27-07 1.08-07 8.83-08 6.34-08 4.83-08 3.66-08
  -1
  -1  -1
C-------------------------------------------------------------------------
C
C  ADAS 2002 preferred data
C  ------------------------
C
```

```
C
C  Source file:  he0_excitation_ionisation_adf04_type1.xls
C
C  Note:  The source file is an automatic linked assembly from component
C  Source directory: /.../adas/adas_excel/he0_electron_impact_xsects
C         workbooks for excitation and ionisation as
C         (1) he0_excitation_1s(1S)-nl().xls
C         (2) he0_excitation_2s(3S)-nl().xls
C         (3) he0_excitation_2s(1S)-nl().xls
C         (4) he0_excitation_2p(1P)-nl().xls
C         (5) he0_excitation_2p(3P)-nl().xls
C         (6) he0_excitation_3s(1S)-nl().xls
C         (7) he0_excitation_3s(3S)-nl().xls
C         (8) he0_excitation_3p(1P)-nl().xls
C         (9) he0_excitation_3p(3P)-nl().xls
C        (10) he0_excitation_3d(1D)-nl().xls
C        (11) he0_excitation_3d(3D)-nl().xls
C        (12) he0_excitation_4s(1S)-nl().xls
C        (13) he0_excitation_4s(3S)-nl().xls
C        (14) he0_excitation_4p(3P)-nl().xls
C        (15) he0_excitation_4d(1D)-nl().xls
C        (16) he0_excitation_4d(3D)-nl().xls
C        (17) he0_excitation_4f(1F)-nl().xls
C        (18) he0_excitation_4f(3F)-nl().xls
C
C        (19) he0_ionisation.xls
C
C         There is no member for 4p(1P) - the highest lying explicit level.
C         The workbooks contain historic comparative assessments of helium
C         data and ADAS preferred data sets.  The workbooks are available to
C         identified data assessors for further study.
C         (see ADAS User Manual version 2.6.
C
C  Compiler:  H. P. Summers, University of Strathclyde
C
C  Date:  14 March 2002
C-----------------------------------------------------------------------
C  Error block
C  -----------
C
C  The value in each error line corresponds to high energy.  Precise meanings
C  are in the ADAS_EXCEL workbooks.
C
C+++ERROR specification start++++++
C
C Ionisation
C
C 1-1    5.0
C 2-1   20.0
C 3-1   20.0
C 4-1   20.0
C 5-1   20.0
C *-1     50.0
C
C Excitation
C
C 1-2    7.7
C 1-3    8.9
C 1-4   31.7
  .       .       .
```

```
C 5-8   19.6
C 5-9    6.2
C 5-10   4.5
C 5-11   1.7
C 6-7    2.9
C 1-*   15.0
C 2-*   15.0
C 3-*   15.0
C 4-*   15.0
C 5-*   15.0
C *-*   30.0
C
C
C
C
C+++ERROR specification end++++++++
C-------------------------------------------------------------------------------
C
C  File generated by converting an ADF04 dataset from type 1 to type 3
C
C  Program     : ADAS809
C
C  Source file : /home/summers/adas/adf04/helike/helike_hps02he_t1.dat
C
C  Producer    : H. P. Summers
C
C  Date        : 18/03/02
C-------------------------------------------------------------------------------

C-------------------------------------------------------------------------------
C ADAS ADF04 DATA - SCCS info: @(#)helike_hpsh02he.dat        1.1 Date 03/22/02
C-------------------------------------------------------------------------------
```