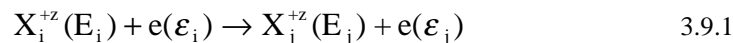


## ADAS209: General level bundling

The program processes specific ion files of type ADF04. The specific ion file is converted to a smaller file of similar organisation according to a level 'bundling' strategy. The output file is of type ADF04 and suitable for direct entry in the user's ADAS database. There is no graphical output.

### Background theory:

Consider the electron impact excitation reaction between two excited levels  $i$  and  $j$ , of an ion  $X^{+z}$ , of an element  $X$ ;



where  $E_i$  ( $E_j$ ) is the excitation energy of level  $i$  ( $j$ ), and  $\varepsilon_i$  ( $\varepsilon_j$ ) is the incident (scattered) electron energy. Then, the Maxwell averaged (effective collision strength) is

$$Y_{ij} = \int_0^{\infty} \Omega_{ij}(\varepsilon_j) \exp(-\varepsilon_j/kT_e) d(\varepsilon_j/kT_e) \quad 3.9.2$$

where  $\Omega_{ij}$  is the collision strength. If we now consider a transition  $I$  to  $J$  in LS coupling then the '*LSJ bundled*' effective collision strength is a summation over the effective collision strengths between  $J$ -resolved fine structure levels, such that,

$$Y_{IJ} = \sum_{i \in I} \sum_{j \in J} Y_{ij} \quad 3.9.3$$

Spontaneous emission coefficients (Einstein A-values) corresponding to the new '*bundled*' transition are given by,

$$A_{J \rightarrow I} = \sum_{i \in I} \sum_{j \in J} \omega_j A_{j \rightarrow i} / \omega_J \quad 3.9.4$$

where,

$$\omega_J = \sum_{j \in J} \omega_j \quad 3.9.5$$

The ADAS209 code makes use of the above expressions in calculating the user selected bundles.

In ionisation and recombination reactions it is proper to distinguish metastable states as potential final states for ionisation and initial states for recombination. In this context, parent states of the  $X^{+z+1}$  ion are identified in advanced format ADF04 files, and these too can be bundled if specific studies require only consideration of the ground states, or, if LSJ parent information is available. Three types of parent metastable information are identified which appear on the first line of the ADF04 file. These are 'term parents' with code '<2S+1>L', 'level parents' with code '<2S+1>L<2J+1>' and unidentified parents '<stat. weight.>'. The latter occur when mixed symmetry metastable parents are combined. In all these cases, the parent energy (relative to the lowest level of the ion) is calculated in the same way as the excitation energy ( $E_i$ ) for each of the levels of  $X^{+z}$ , namely,

$$E_{J \rightarrow I} = \sum_{i \in I} \sum_{j \in J} \omega_j E_{j \rightarrow i} / \omega_J - E_{\text{shift}} \quad 3.9.6$$

where  $E_{\text{shift}}$  is the relative change in energy between the lowest states of  $X^{+z}$  and  $X^{+z+1}$  and is therefore zero for all excited levels of  $X^{+z}$ .

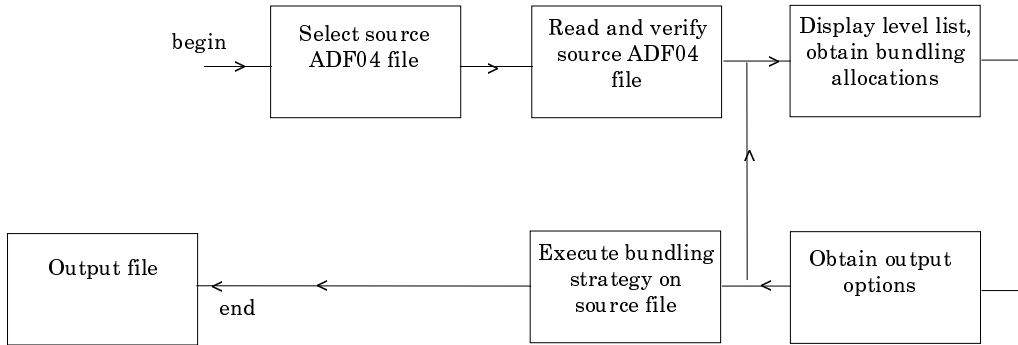
The code is arranged to be quite flexible in its bundling strategy in that any levels may be grouped. However this can lead to difficulties when levels of different symmetries and configurations are bundled. This is especially the case when the levels of such a bundle span a target state for spontaneous emission from or to the bundle. A warning is issued by the code in these circumstances. It is essential to look at the output ADF04 file in such cases since spurious Einstein coefficients may be inserted and the same transition may appear twice but

with upper and lower bundle indices interchanged. In fact these correspond to the upward and downward division. The safest strategy is usually to delete the spontaneous coefficients and add the Upsilon's.

### Program steps:

These are summarised in figure 3.9.

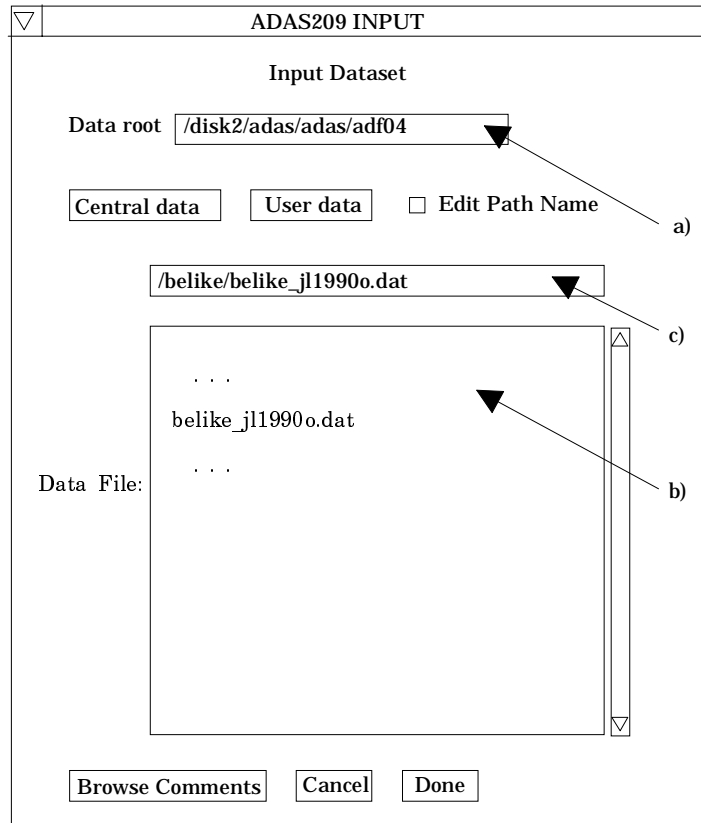
Figure 3.9



### Interactive parameter comments:

Programs of this series (ADAS2) which make use of data from archived ADAS datasets initiate an interactive dialogue with the user in three parts, namely, input file selection, entry of user data and disposition of output.

The **file selection window** has the appearance shown below

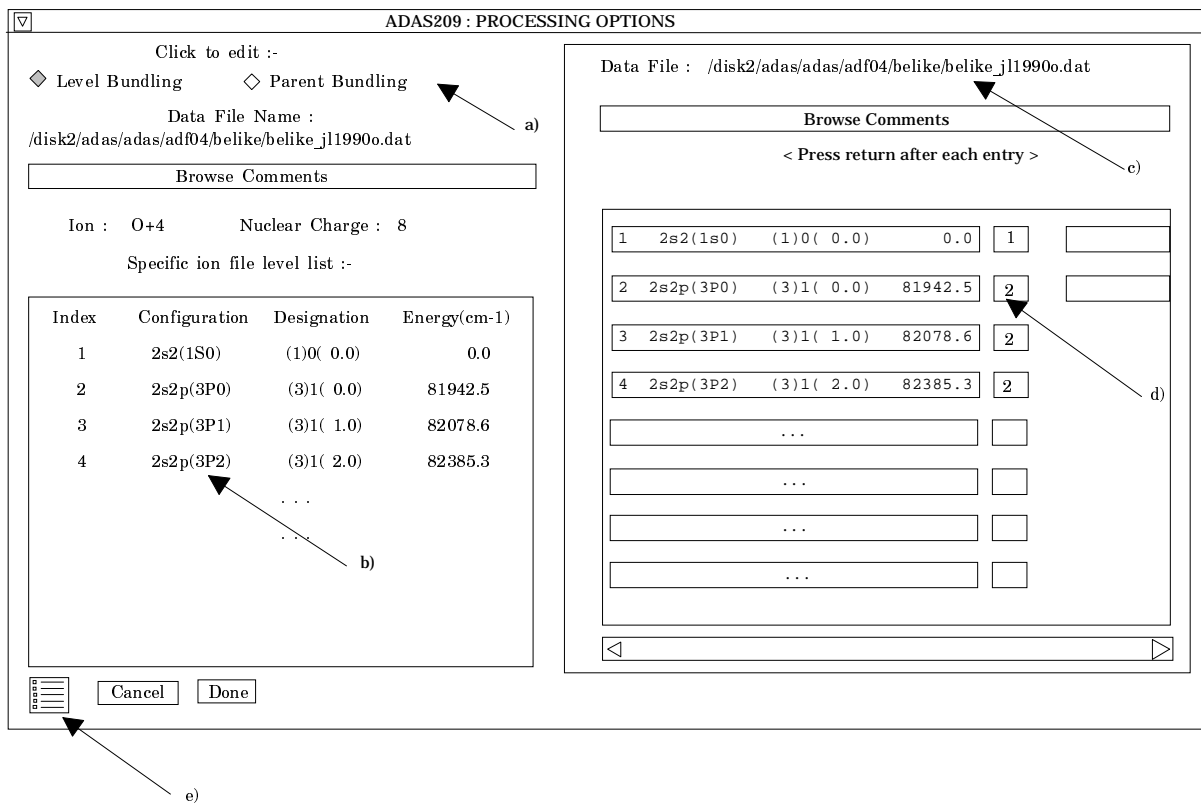


1. Data root a) shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. The appropriate ADAS data format for input to this program is ADF04 ('specific ion files'). Click the *User Data* button to insert the pathway to your

own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*, to use this facility.

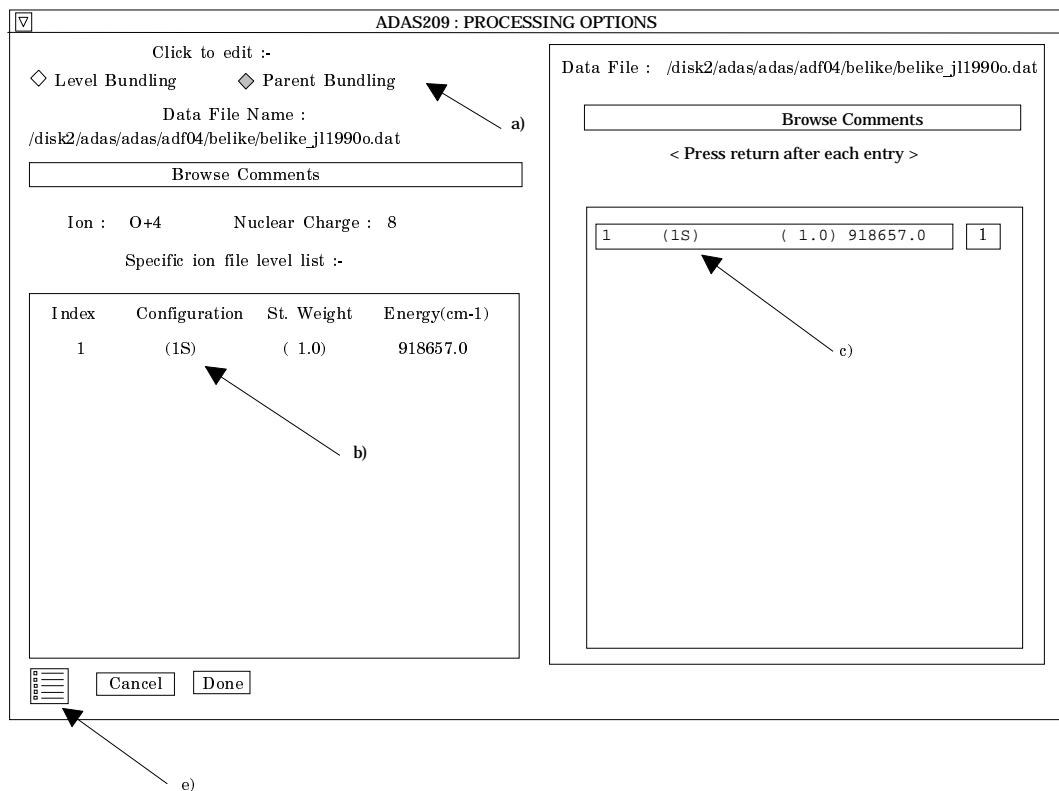
2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
3. Available sub-directories are shown in the large file display window b). Scroll bars appear if the number of entries exceed the file display window size.
4. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
5. Once a data file is selected, the set of buttons at the bottom of the main window become active.
6. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.
7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

The processing options window has the appearance shown below



8. At a), two buttons are present to allow bundling of the levels of the selected ion and then bundling of the parents of these levels. The parents are the ground and metastable levels of the next higher ion to which ionisation may take place or from which recombination may take place. For basic studies, you will probably be using ADF04 datasets which omit recombination and assume ionisation only to the ground state of the next higher ion. Then the subtleties of parents may be ignored. This parent bundling option is non-trivial only when the advanced ADF04 specification is being used. Click the appropriate button to fill the left side level display window b) and the right side Bundling window d).
9. The level list displayed in the window at a) is for information only and is a simple transcription of the list from the head of the source ADF04 file.

10. Note that the Data File Name at the left side is the same as the Data file at c) on the right side.
11. In the Level Bundling window, the index number, configuration specification,  $(2S+1)L(J)$  quantum numbers and the level energy (cm-1) are given for each level in a separate display window with an editable box to its right d). The editable box is for entering a bundle index number. That is levels which are to be grouped are given the same bundle index number. If no index number is given for a level, then the code treats the level as a distinct bundle. The code re-indexes bundles as necessary for consistency. **Remember to press Return after entering each bundle index.**
12. When you have finished the level bundling allocation, click the *Parent Bundling* button at a) to execute parent bundling. Note you may proceed to the next screen directly by clicking the *Done* button after level bundling. The code then puts in the default parent.
13. On clicking the Parent Bundling button the windows at b) and d) are filled with the corresponding parent information. The display is illustrated below. It generally has less than five entries and if the advanced ADF04 format is not in use then only one. The information format is a little different from that of the levels. The first value is the index number, followed by the parent term character string (in brackets) as given on the top line of the ADF04 file. The numerical value of the parent statistical weight follows with finally the parent energy (cm-1) relative to the lowest level of the ion. In the single parent case therefore this is just the ionisation potential.



14. Note that the organisation of all ADF04 datasets at present is such that although energy levels may be at the J-resolved intermediate coupling resolution, the parents are at term resolution. Thus there is usually no need to bundle parents unless there is a wish to focus for example on just the ground parent (lowest ionisation continuum). The latter may be the case if one wishes to bypass the complexities of metastables. ADAS209 does however have the capability of dealing specifically with J-resolved parents.
15. Note the icon for *Exit to Menu* at (e). This quits the program and returns you to the ADAS series 2 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen

The **output options window** is of restricted form. It only offers the option of an output file. This part is of the same layout as codes previously described.

16. The name of the source data file which has been bundled is repeated at a) for information. The output file is the bundled ADF04 file and it is of the correct format for re-entry in the ADF04 database. However, if you have used the defaults on parent bundling, it is advisable to check the top line of the file to see that the term allocation of the ground state is what you wish. The comments section at the end of the output ADF04 file details the source ADF04 file and the bundling imposed.

17. By default the output file is sent to your */pass* file subdirectory as *bundle.pass*. You should ensure that you have created a */pass* sub-directory of you personal */adas* directory to receive such files.

18. There is no graphical output option.

### Illustration:

Table 3.9a shows the input ADF04 file for  $O^{+4}$  in LSJ-resolution. Table 3.9b shows the bundled ADF04 file resulting from combining levels of the same triplet terms. Note that the bundled groups are distinguished by a "\*" and that the configuration name is simply that of the first level which enters the bundle. Note that on the top line the parent term is a default one '(1S)' since the original source file contained no details of the ground state parent but only its ionisation potential. In the comments section at the end of the data, the bundling details are recorded by giving the *Original level indexing* and the *Selection vector*. Note that the *Parent bundling vector* is '0' recognising that no parent bundling was done.

Table 3.9a

O + 4	8	5	918657.						
1	2S2(1S0)	(1)0( 0.0)	0.0						
2	2S2P(3P0)	(3)1( 0.0)	81942.5						
3	2S2P(3P1)	(3)1( 1.0)	82078.6						
4	2S2P(3P2)	(3)1( 2.0)	82385.3						
5	2S2P(1P1)	(1)1( 1.0)	158797.7						
6	2P2(3P0)	(3)1( 0.0)	213462.5						
7	2P2(3P1)	(3)1( 1.0)	213618.2						
8	2P2(3P2)	(3)1( 2.0)	213887.0						
9	2P2(1D2)	(1)2( 2.0)	231721.4						
10	2P2(1S0)	(1)0( 0.0)	287910.3						
11	2S3S(3S1)	(3)0( 1.0)	546972.7						
12	2S3S(1S0)	(1)0( 0.0)	561276.4						
13	2S3P(1P1)	(1)1( 1.0)	580824.9						
14	2S3P(3P0)	(3)1( 0.0)	582806.4						
15	2S3P(3P1)	(3)1( 1.0)	582843.1						
16	2S3P(3P2)	(3)1( 2.0)	582920.3						
17	2S3D(3D1)	(3)2( 1.0)	600748.9						
18	2S3D(3D2)	(3)2( 2.0)	600758.9						
19	2S3D(3D3)	(3)2( 3.0)	600779.2						
20	2S3D(1D2)	(1)2( 2.0)	612615.6						
-1									
5.00	3	2.50+04	5.00+04	1.25+05	2.50+05	5.00+05	1.25+06	2.50+06	5.00+06

```

3 1 2.17+03 2.04-01 1.80-01 1.50-01 1.27-01 1.02-01 6.81-02 4.55-02 2.75-02
4 1 2.16-02 3.40-01 2.99-01 2.49-01 2.11-01 1.70-01 1.14-01 7.59-02 4.59-02
. . . . .
16 15 1.00+30 6.79+00 6.90+00 5.43+00 4.29+00 3.46+00 2.27+00 1.55+00 1.08+00
18 17 1.00-30 2.10+00 2.17+00 2.03+00 1.74+00 1.38+00 8.94-01 6.00-01 3.82-01
19 17 1.00-30 1.55+00 1.57+00 1.25+00 9.33-01 6.54-01 3.85-01 2.52-01 1.62-01
19 18 1.00-30 3.30+00 3.26+00 2.90+00 2.41+00 1.85+00 1.17+00 7.79-01 4.93-01
-1
-1 -1
-----
C
C
C The effective collision strengths are calculated using the fit
C parameters of Kato,Lang,& Berrington 1990 (Atomic Data and Nuclear
C Data Tables 44,133),and the analytical formulae (3 & 4) therein.
C
C The data for transition probabilities among the n=2 and n=3 levels
C
C 15-18 to 11.9%, 16-18 to 14.9%, 6-14 to 15.4%, 15-19 to 13.9%
C 8-14 to 18.9%, 17-18 to 22.7%, 18-19 to 25%, 6-8 to 38%,
C 7-8 to 52.7%
C In fact the alterations have accentuated the differences between
C the 1990 & 1994 data for the 6-8,7-8 transitions. The comments on
C this comparison (above) are unaffected.
C
C
C D.H.Brooks 16.08.95
-----

```

Table 3.9b

```

O + 4      8      5 918657.0(1S)
1 2S2(1S0)      (1)0( 0.0)      0.0 {1}1.000
2 2S2P(3P0)    *(3)1( 4.0)      82233.9 {1}1.000
3 2S2P(1P1)    (1)1( 1.0)      158797.7 {1}1.000
4 2P2(3P0)     *(3)1( 4.0)      213750.2 {1}1.000
5 2P2(1D2)     (1)2( 2.0)      231721.4 {1}1.000
6 2P2(1S0)     (1)0( 0.0)      287910.3 {1}1.000
7 2S3S(3S1)    (3)0( 1.0)      546972.7 {1}1.000
8 2S3S(1S0)    (1)0( 0.0)      561276.4 {1}1.000
9 2S3P(1P1)    (1)1( 1.0)      580824.9 {1}1.000
10 2S3P(3P0)   *(3)1( 4.0)      582881.9 {1}1.000
11 2S3D(3D1)   *(3)2( 7.0)      600766.4 {1}1.000
12 2S3D(1D2)   (1)2( 2.0)      612615.6 {1}1.000
-1
5.00      3      2.50+04 5.00+04 1.25+05 2.50+05 5.00+05 1.25+06 2.50+06 5.00+06
2 1 7.23+02 6.12-01 5.39-01 4.49-01 3.80-01 3.06-01 2.05-01 1.37-01 8.26-02
3 1 2.86+09 2.63+00 2.67+00 2.81+00 3.02+00 3.36+00 4.03+00 4.68+00 5.44+00
4 1 1.87-01 9.33-03 1.08-02 1.20-02 1.16-02 9.92-03 6.84-03 4.65-03 2.95-03
5 1 2.96+03 1.10-01 1.13-01 1.17-01 1.16-01 1.10-01 9.09-02 7.28-02 5.54-02
. . . . .
11 4 3.00-30 2.13+00 1.85+00 1.33+00 9.09-01 5.53-01 2.55-01 1.38-01 7.50-02
11 10 3.00-30 5.25+01 5.70+01 8.07+01 1.06+02 1.32+02 1.61+02 1.77+02 1.89+02
-1
-1 -1
-----
C
C
C File generated by compression of a J-resolved file
C
C Program: ADAS209
C
C Source file: /packages/adas/adas/adf04/belike/belike_jl1994o.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 0 1 1 1 0 2 2 2 0 0
C 0 0 0 3 3 3 4 4 4 0
C
C Original parent metastables:
C (1S)
C Parent bundling vector:
C 0
C
C Producer: Stuart Loch
C Date: 11/03/99
-----

```

**Notes:**