Atomic Data and Analysis Structure

Coping with large quantities of data

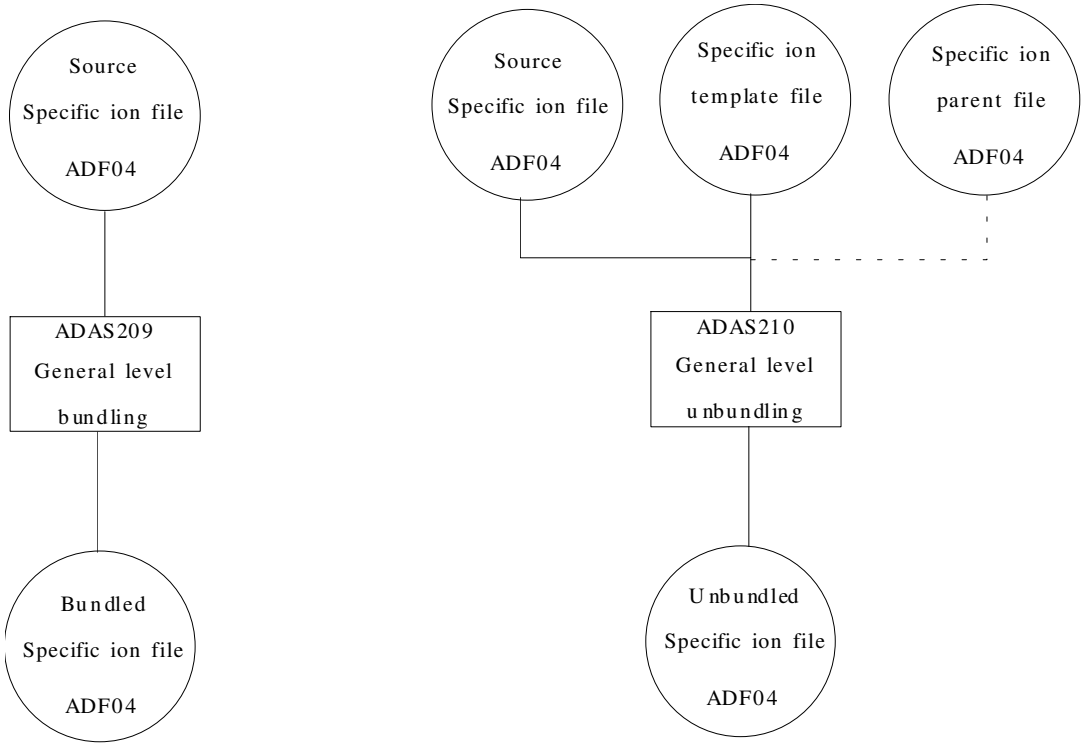
The programs in this group belong to series ADAS2 and both are interactive processing codes on elements of the fundamental database. A schematic of the programs and dataset types interrogated is shown in figure 5.0. Each program extracts specific ion file data from the relevant data collection, acquires information from the user on his/her stategy for associating levels and then outputs the modified data set. No graphical display is produced. The output datasets are organised for direct entry into the user's personal ADAS fundamental database.

ADAS209 is designed to help with the problem of being overwhelmed with data when studying the excited populations and emissivities of complex ions. One seeks to simplify by grouping excited populations of similar levels or of levels of minor importance. We call this 'working at different resolution levels' in excited population structure. A specific situation is that in astrophysical studies where intermediate coupling LSJ resolution of populations is usual, even for light species, to assist high resolution spectroscopy. From the population structure point of view LS resolution is adequate. In fusion, LS resolution is usual for light species. The new code allows controlled 'bundling' of level populations. It does this by operating on a specific ion file (type ADF04) of high resolution and generating a new file of the same type but of lower resolution as prescribed by the user. Such an algorithm is also of value with very many level systems where there is a need to focus on the most important levels, for example metastables, and treat other levels more grossly.

ADAS210 is designed to help with the problem of handling data when studying the excited populations and emissivities of ions at different degrees of fineness (resolution levels) in excited population structure. One seeks to change between resolution levels easily. The astrophysical example is again apposite. One may have data of high quality at LS resolution for some ions which it is desired to convert to LSJ resolution for special studies. The new code allows controlled 'unbundling' of level populations. It does this by operating on a specific ion file (type ADF04) of low resolution and generating a new file of the same type but of higher resolution as prescribed by the user. Such a procedure is of course not a substitute for original high resolution cross-section data. However the procedure tries to maintain precision by using a 'template' file of high resolution (also of type ADF04) to aid in the 'unbundling' of the low resolution source ADF04 file.

Such algorithms are also of value with very many level systems where there is a need to focus on the most important levels perhaps at high resolution while treating other levels more grossly.

Figure 5.0


Source
Specific ion file
ADF04
ADAS209
General level
bundling
Bundled
Specific ion file
ADF04
Source
Specific ion file
ADF04
Specific ion
template file
ADF04
Specific ion
parent file
ADF04
ADAS210
General level
unbundling
Unbundled
Specific ion file
ADF04

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' stategy. The output file is 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*;

$$X_i^{+z}(E_i) + e(\varepsilon_i) \rightarrow X_j^{+z}(E_j) + e(\varepsilon_j) \qquad 5.9.1$$

where E_i (E_j) is the exitation energy of level i(j), and ε_i (ε_j) is the incident (scattered) electron energy.Then, the Maxwell averaged (effective colllision strength)

$$\gamma_{ij} = \int_0^\infty \Omega_{ij}(\varepsilon_j)\exp(-\varepsilon_j/kT_e)\, d(\varepsilon_j/kT_e) \qquad 5.9.2$$

where Ω_{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,

$$\gamma_{IJ} = \sum_{i\in I}\sum_{j\in J}\gamma_{ij} \qquad 5.9.3$$

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

$$A_{J\rightarrow I} = \sum_{i\in I}\sum_{j\in J}\omega_j A_{j\rightarrow i}/\omega_J \qquad 5.9.4$$

where,

$$\omega_J = \sum_{j\in J}\omega_j \qquad 5.9.5$$

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,

$$E_{J\rightarrow I} = \sum_{i\in I}\sum_{j\in J}\omega_j E_{j\rightarrow i}/\omega_J - E_{shift} \qquad 5.9.6$$

where E_{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}.

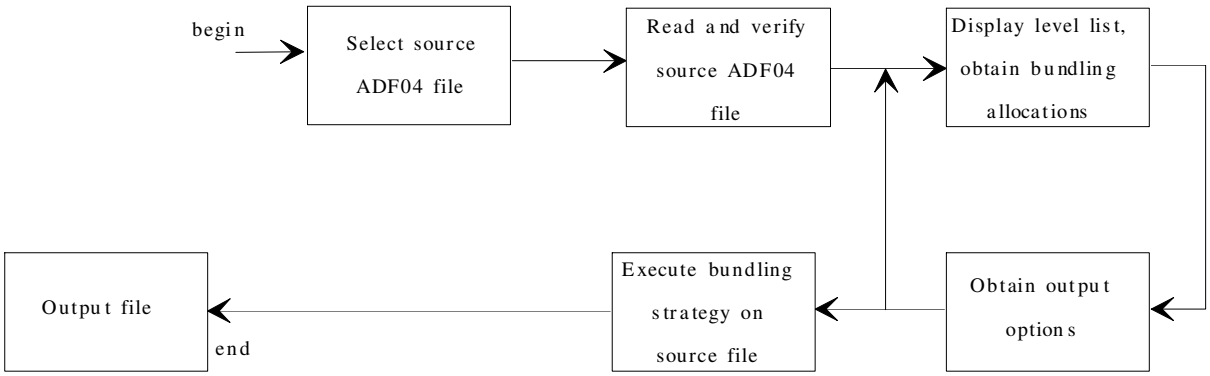
The code is arranged to be quite flexible in its bundling strategy in that any levels may be grouped. However this can lead to difficulties when levels of different symmetries and configurations are bundled. This is especially the case when the levels of such a bundle span a target state for spontaneous 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 uppward and downward division. The safest stategy is usually to delete the spontaneous coefficients and add the upsilons.

Program steps:

These are summarised in figure 5.9.

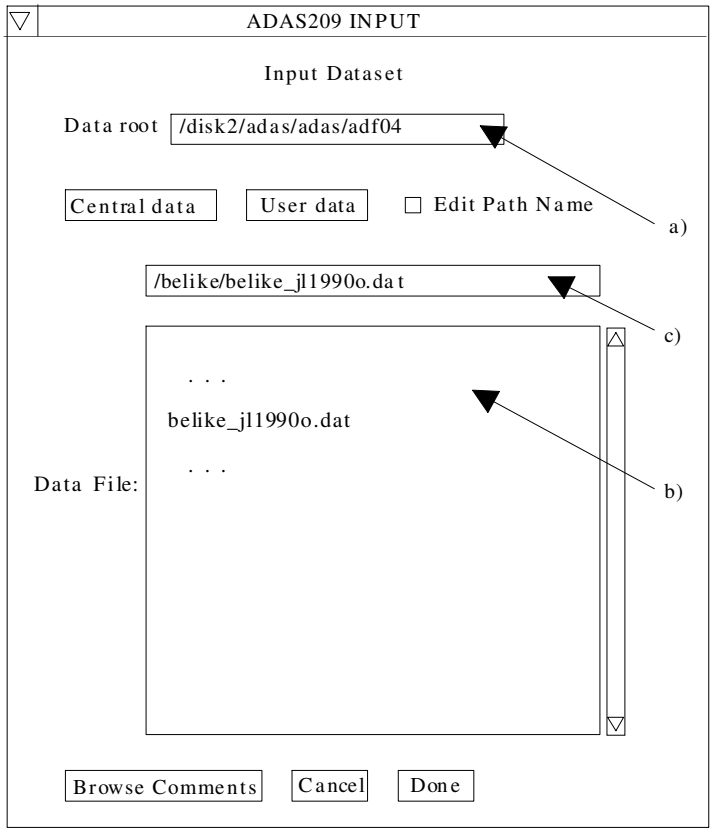
Figure 5.9



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

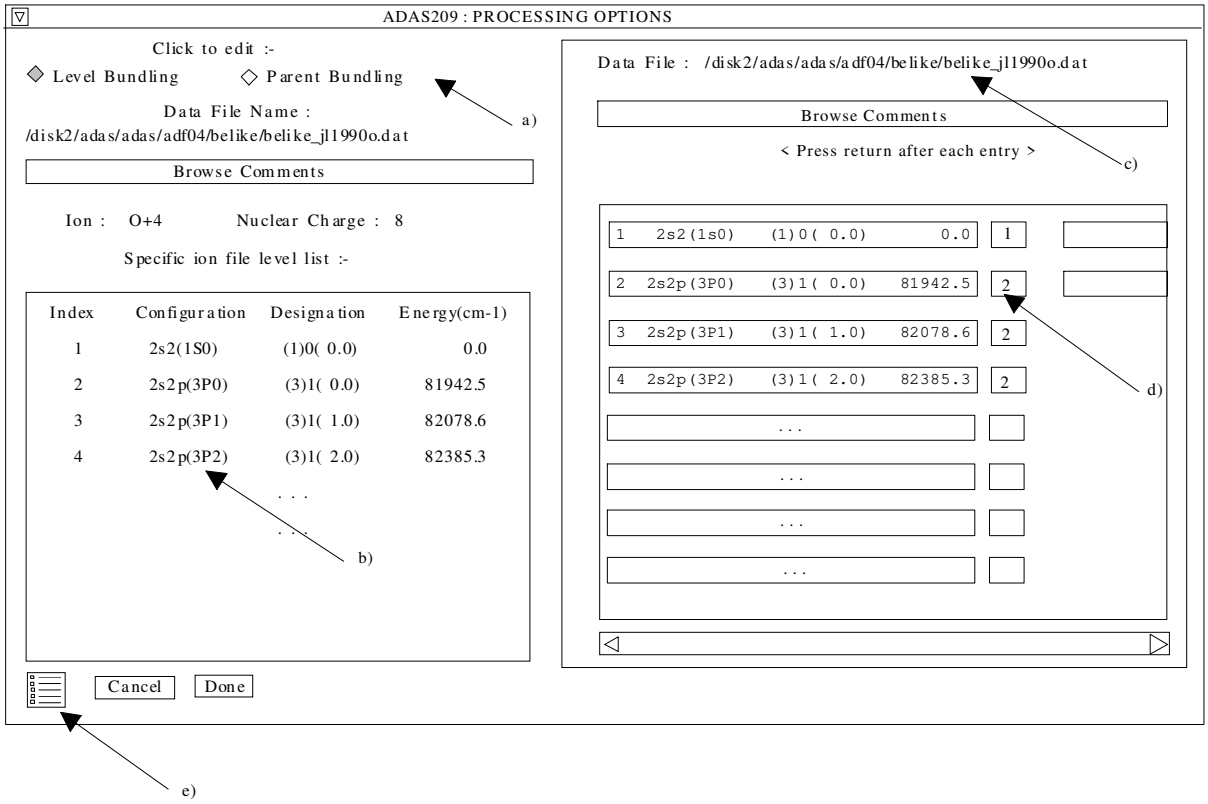


1. Data root a) shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the

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. More details are given in the ADAS Manual. Click the appropriate button to fill the left side level display window b) and the right side Bundling window d).

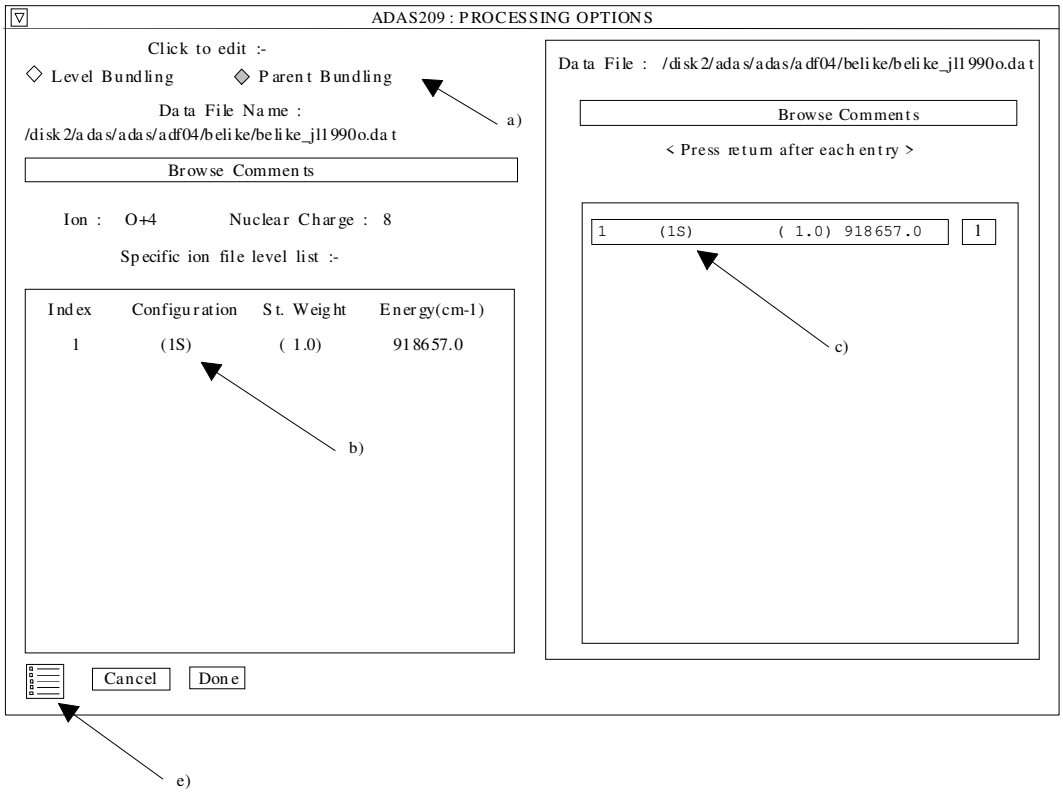
9. The level list displayed in the window at a) is for information only and is a simple transcription of the list from the head of the source ADF04 file.

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 reindexes 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.



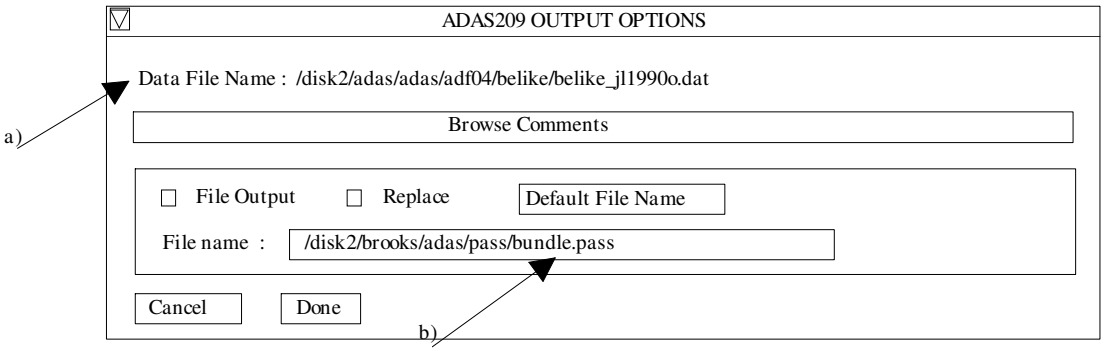
14. Note that the organisation of all ADF04 datasets at present is such that although energy levels may be at the J-resolved intermediate coupling resolution, the parents are at term resolution. Thus there is usually no need to bundle parents

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.

Figure 5.9d



1. 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.
2. 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.
3. There is no graphical output option.

Illustration:

Figure 5.9a shows the input ADF04 file for O^{+4} in LSJ-resolution. Figure 5.9b 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 5.9a

```
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
   2   1 1.00-30 6.79-02 5.99-02 4.99-02 4.23-02 3.40-02 2.27-02 1.52-02 9.18-03
   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 7.74+00 6.90+00 5.43+00 4.29+00 3.26+00 2.17+00 1.55+00 1.09+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    15-18 to 11.9%, 16-18 to 14.9%, 6-14  to 15.4%, 15-19 to 15.9%
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                                       D.H.Brooks 16.08.95
C-----------------------------------------------------------------------
```

Table 5.9b

```
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   2 6.85+10 3.30+00 3.30+00 3.33+00 3.46+00 3.78+00 4.56+00 5.41+00 6.42+00
  10   4 5.27+07 2.09+00 1.79+00 1.21+00 7.72-01 5.35-01 7.72-01 1.32+00 2.00+00
  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: /home/brooks/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
C  Insert producer id here: D.H.Brooks
C  Date: 19/01/96
C
C-------------------------------------------------------------------------------
```

Notes:

ADAS210: General level unbundling

The program processes specific ion files of type ADF04. The specific ion source file is converted to a larger file of similar organisation according to a level 'unbundling' stategy. A template file of type ADF04 must also be available to support the processing. 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*;

$$X_I^{+z}(E_I) + e(\varepsilon_I) \rightarrow X_J^{+z}(E_J) + e(\varepsilon_J) \qquad 5.10.1$$

where E_I (E_J) is the excitation energy of level *I*(*J*), and ε_I (ε_J) is the incident (scattered) electron energy. If we have high precision calculation data for the effective collision strength associated with this transition, we may wish to obtain an *'LSJ unbundled'* effective collision strength corresponding to the fine structure transition, $i \in I$ to $j \in J$, in LSJ intermediate coupling. In ADAS210 we use two methods to do this. First, we may already have lower quality data at LSJ resolution. If so, we can use ADAS209 to bundle this data and then form a ratio with our new data to use as a premultiplier to our lower quality data i.e. we normalise the J proportions of the lower quality, to that of the higher quality data. Therefore,

$$\gamma_{ij}^{Jn} = \gamma_{ij}^{Jo}\, \gamma_{IJ}^{LS} / \gamma_{IJ}^{BLSJ} \qquad 5.10.2$$

where γ_{ij}^{Jn} denotes the new LSJ effective collision strength, γ_{ij}^{Jo}denotes the lower quality LSJ value, γ_{IJ}^{LS} is the high quality LS resolved value and γ_{IJ}^{BLSJ} is the bundled lower quality values and is given by,

$$\gamma_{IJ}^{BLSJ} = \sum_{i \in I} \sum_{j \in J} \gamma_{ij} \qquad 5.10.3$$

The spontaneous emission coefficients (Einstein A-values), can be calculated in a similar manner such that,

$$A_{j \rightarrow i}^{Jn} = A_{j \rightarrow i}^{Jo} \left(A_{J \rightarrow I}^{LS} / A_{J \rightarrow I}^{BLSJ} \right) \omega_J^{LS}, \qquad 5.10.4$$

where,

$$A_{J \rightarrow I}^{BLSJ} = \sum_{i \in I} \sum_{j \in J} A_{j \rightarrow i}\, \omega_j^{Jo} / \omega_J^{BLSJ} \qquad 5.10.5$$

with *Jo* and *Jn* referring to lower quality J-resolved data and new data respectively and superscript LS referring to the higher quality LS resolved data. In this case, the statistical weights have been included with analogous markings, and

$$\omega_J^{BLSJ} = \sum_{j \in J} \omega_j^{Jo} \qquad 5.10.6$$

Secondly, if we do not have any LSJ data, we use statistical splitting which gives

$$\gamma\left({}^{2S+1}L_J, {}^{2S'+1}L_{J'}\right) = \sum_J \sum_{J'} \left(\frac{2J+1}{(2L+1)(2S+1)} \right) \left(\frac{2J'+1}{(2L'+1)(2S'+1)} \right) \gamma\left({}^{2S+1}L, {}^{2S'+1}L'\right) \qquad 5.10.7$$

The *A*-values are zeroed in this case.

Parent problems

In ionisation and recombination reactions it is proper to distinguish metastable states as well as ground states as potential final states for ionisation and initial states for recombination. For this reason, parent states of the X^{+z+1} ion are identified in the advanced format form of ADF04 files. These parents drive the population structure calculations and should be

included explicitly in any ionisation balance. For light ions LS term resolution of metastable parents is adequate but a move to intermediate coupling may be required for highly ionised ions. This may also assist in high resolution spectroscopy. Consistency between resolution levels in fundamental and derived data is desirable. Bundling and unbundling allows us to 'work at different resolution levels'. ADAS210 can handle the unbundling of recombining ion parent metastables as well as the usual bound excited states of the recombined ion.

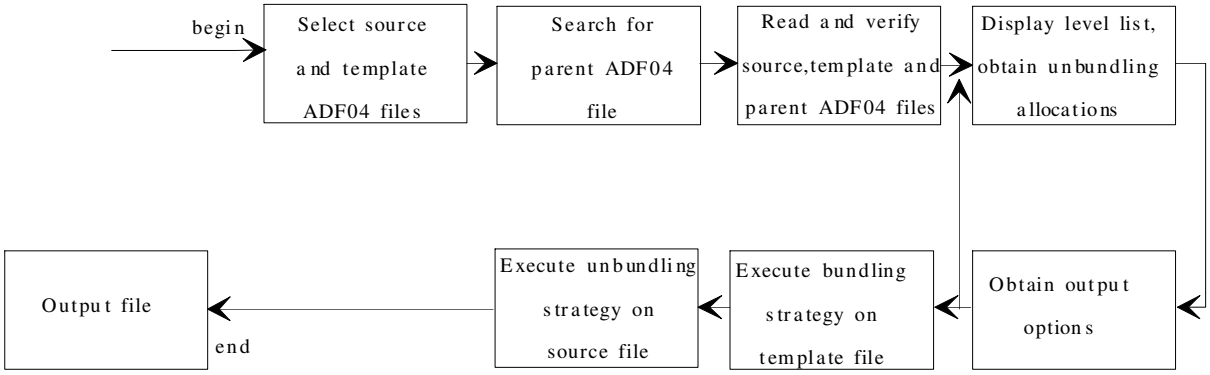
In unbundling, an additional template parent dataset at LSJ resolution is required and located by a search mechanism in ADAS210. If available, the parent configurations, parent energies and statistical weights are transcribed from the template following the selections entered by the user. Three types of parent metastable information are identified which appear on the first line of the source 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.The energies are always adjusted to account for the energy shift relative to the lowest level of the ion. Only these forms are recognised by the subroutines which read ADF04 files.

In these cases the advanced specification ADF04 files are in use. Such files include information about the effective contributions to ionisation from each of the levels to each of the parent metastables (for more information see the description of ADAS208 in the last chapter of this manual and the specification of the ADF04 format in the Appendix).

Program steps:

These are summarised in figure 5.10.

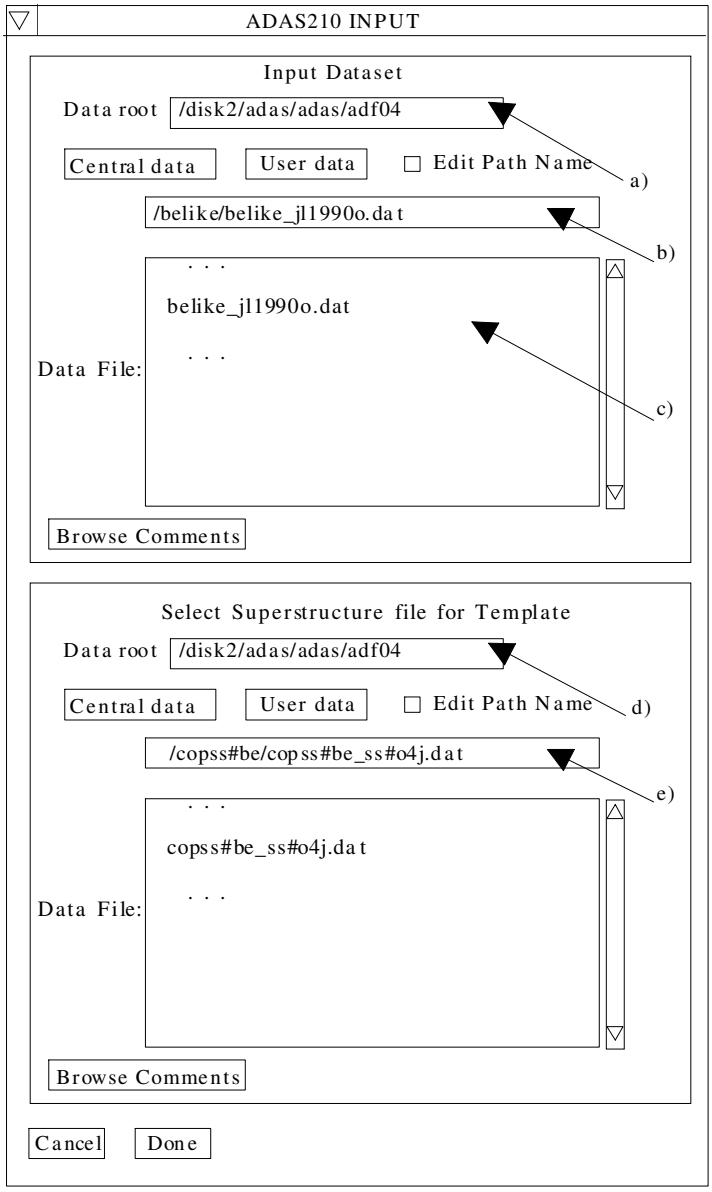
Figure 5.10



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



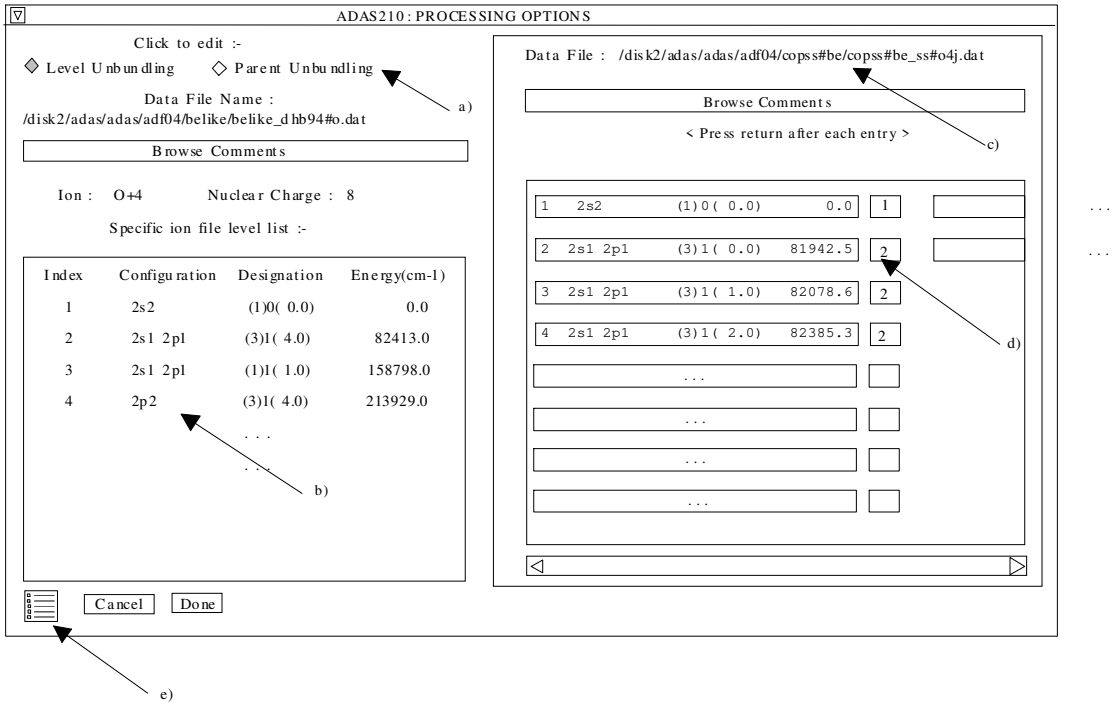
1. Selection of the source file to be unbundled is made in the top window. Data root a) shows the full pathway to the appropriate data subdirectories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. The appropriate ADAS data format for input to this 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 c). 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 b) 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 the data files are 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. Selection of the 'template' file which assists in the unbundling is made in the lower window at d) and e) as for the source file. The information line refers to a 'Superstructure file' as template. We have mass produced such files at high resolution and they provide a good starting point. It is not obligatory to use an ADF04 file produced from the 'Superstructure' code as a template, but it must be drawn from a data collection with the same detailed naming conventions as the Superstructure collections. Incidentally such files are held in their own subdirectories of the /ADF04 directory according to isoelectronic sequence. Look for the code letter '*j*' at the end of the ion name to tell you that the file is of high (ie. LSJ) resolution (eg. */.../adas/adas/adf04/copss#be/copss#be_ss#o4j.dat*).

8. Clicking the *Done* button moves you forward to the next screen. Clicking the *Cancel* button takes you back to the previous screen

The **processing options window** has the appearance shown below



1. At a), two buttons are present to allow unbundling of the levels of the selected ion and then unbundling 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 unbundling option is non-trivial only when the advanced ADF04 specification is being used. More details are given in the ADAS Manual. Click the appropriate button to fill the left side level display window b) and the right side Unbundling window d).

2. The level list displayed in the window at b) is from the source file which is to be unbundled and is for information only. It is a simple transcription of the list from the head of the source ADF04 file.

3. Note that the Data File at the right hand side c) is the template file.

4. In the Level Unbundling 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 the index number of the source file level which you wish to associate with the high resolution template file level. Essentially the template levels are bundled first in the procedure for association with the low resolution source levels. That is template levels which are to be grouped are given the index number of their associated low resolution source file level. Then the low resolution level is unbundled in the proportions of the template file levels forming the group. **Remember to press Return after entering each associated level index**.

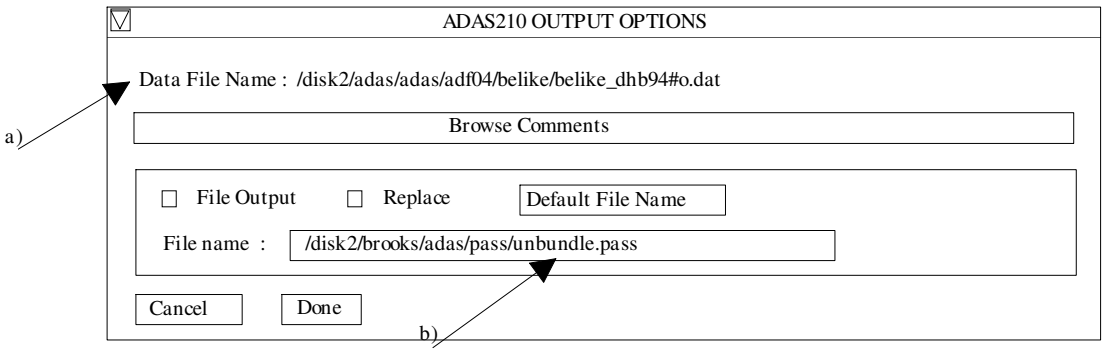
5. When you have finished the level allocation, click the *Parent Unbundling* button at a) to execute parent bundling. Note you may proceed to the next screen directly by clicking the *Done* button after level unbundling, but in this case a default '(1S)' parent is introduced. In this circumstance it is advisable to check that the top line of the output specific ion file is consistent with your intentions.

6. On clicking the Parent Unbundling button the window at b) is filled with the parent information from the source file. The window at d) by contrast is filled with level information from a template file for the adjacent higher ion of the same sub-directory class as the template file for the level unbundling. Thus if *'/.../adas/adas/adf04/copss#be/copss#be_ss#o4j.dat'* was the level template then *'/.../adas/adas/adf04/copss#li/copss#li_ss#o5j.dat'* is the parent template. 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.

7. 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. The parent subject is of some depth and more details are given in the ADAS User Manual. For basic studies, these issues may be ignored.

8. 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.



9. The name of the source data file which has been unbundled is repeated at (a) for information. The output file is the unbundled ADF04 file and it is of the correct format for re-entry in the ADF04 database. The comments section at the end of the output ADF04 file details the source ADF04 file and the unbundling imposed.

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

11. There is no graphical output option.

Illustration:

An example of a source data set for unbundling is given in figure 5.10a and the unbundled output ADF04 file in figure 5.10b. The source sample here is in fact a bundled file from a prior ADAS209 run. In the comments section at the end of the unbundled data file, the un bundling details are recorded by giving the *Template file indexing* and the *Source file assignment*. Note that the *Parent unbundling vector* is blank recognising that no parent unbundling was done in this case. On the top line of the unbundled file '(1S)' is entered by default.

Table 5.10a

```
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
                                      . . .
  10   2 9.61+05 2.50+00 2.28+00 1.91+00 1.67+00 1.55+00 1.49+00 1.40+00 1.23+00
  11   2 6.85+10 3.30+00 3.30+00 3.33+00 3.46+00 3.78+00 4.56+00 5.41+00 6.42+00
  10   4 5.27+07 2.09+00 1.79+00 1.21+00 7.72-01 5.35-01 7.72-01 1.32+00 2.00+00
  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    LS bundled data set,reassembled from the J-resolved data set
C  'belike_jl1994o.dat'.
C    This was done using a program suitable only for OV but which is currently
C  being altered to work for any data set.It sums level gammas over the
C  relevant term,renumbers the indexing and recalculates the energies and A
C  values.
C
C    All the corrections and comments in 'belike_jl1994o.dat' also apply to
C  this dataset.
C
C    The output A values match those of belike_wjd92#o.dat,except for the
C  ones calculated from superstructur using the same J-resolved A values (from
C  belike_jl1990o.dat)
C
C                                                  D.H.Brooks 9.11.94
C-------------------------------------------------------------------------------
C
C  File generated by compression of a J-resolved file
C
C  Program: ADASDEV
C
C  Source file: /home/brooks/sunadas/belike/jl1994o.dat
C
C  Cross-reference file: None
C  IDL interface: b9ispf.pro (adas209)
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
C  Insert producer id here: D.H.Brooks
C  Date: 16/08/95
C
C-------------------------------------------------------------------------------
```

Table 5.10b

```
O + 4         8         5   918657.0(1S)
    1 2s2                (1)0( 0.0)        0.0
    2 2s1 2p1            (3)1( 0.0)    82544.5
    3 2s1 2p1            (3)1( 1.0)    82698.1
    4 2s1 2p1            (3)1( 2.0)    83007.2
    5 2s1 2p1            (1)1( 1.0)   168195.9
    6 2p2                (3)1( 0.0)   215600.0
    7 2p2                (3)1( 1.0)   215755.1
    8 2p2                (3)1( 2.0)   216059.3
    9 2p2                (1)2( 2.0)   239295.5
   10 2p2                (1)0( 0.0)   300329.8
   11 2s1 3s1            (3)0( 1.0)   545969.0
   12 2s1 3s1            (1)0( 0.0)   562088.2
   13 2s1 3p1            (1)1( 1.0)   581234.9
   14 2s1 3p1            (3)1( 0.0)   582531.6
   15 2s1 3p1            (3)1( 1.0)   582569.6
   16 2s1 3p1            (3)1( 2.0)   582640.4
   17 2s1 3d1            (3)2( 1.0)   601247.4
   18 2s1 3d1            (3)2( 2.0)   601262.9
   19 2s1 3d1            (3)2( 3.0)   601286.1
   20 2s1 3d1            (1)2( 2.0)   616042.1
  -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 6.12-01 5.39-01 4.49-01 3.80-01 3.06-01 2.05-01 1.37-01 8.26-02
   5   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
                    . . .
18  15 2.26-30 1.31+01 1.42+01 2.01+01 2.65+01 3.30+01 4.02+01 4.42+01 4.72+01
  18  16 7.44-31 4.38+00 4.75+00 6.74+00 8.84+00 1.10+01 1.34+01 1.47+01 1.57+01
  19  16 3.00-30 2.45+01 2.67+01 3.77+01 4.95+01 6.17+01 7.52+01 8.28+01 8.83+01
  -1
  -1  -1
C-------------------------------------------------------------------------------
C
C  File generated by expansion of an LS-resolved file
C
C  Program: ADAS210
C
C  Source file: /home/brooks/adas/adf04/belike/belike_dhb94#o.dat
C  Template file:
C  /home/brooks/adas/adf04/copss#be/copss#be_ss#o4j.dat
C
C  Template File indexing:
C     1    2    3    4    5    6    7    8    9   10
C    11   12   13   14   15   16   17   18   19   20
C    21   22   23   24   25   26   27   28   29   30
C    31   32   33   34   35   36   37   38   39   40
C    41   42   43   44   45   46
C  Source File Assignment:
C     0    2    2    2    0    4    4    4    0    0
C     0    0    0   10   10   10   11   11   11    0
C     0    0    0    0    0    0    0    0    0    0
C     0    0    0    0    0    0    0    0    0    0
C     0    0    0    0    0    0
C
C  Original parent metastables:
C
C  Parent unbundling vector:
C
C
C
C  Insert producer id here:
C  Date: 19/01/96
C
C-------------------------------------------------------------------------------
```

Notes: