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*;

$$X_I^{+z}(E_I) + e(\varepsilon_I) \rightarrow X_J^{+z}(E_J) + e(\varepsilon_J) \qquad 3.10.1$$

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 pre-multiplier to our lower quality data i.e. we normalise the J proportions of the lower quality, to that of the higher quality data. Therefore,

$$Y_{ij}^{Jn} = Y_{ij}^{Jo}\, Y_{IJ}^{LS} \big/ Y_{IJ}^{BLSJ} \qquad 3.10.2$$

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

$$Y_{IJ}^{BLSJ} = \sum_{i \in I} \sum_{j \in J} Y_{ij} \qquad 3.10.3$$

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

$$A_{j \rightarrow i}^{Jn} = A_{j \rightarrow i}^{Jo} \left(A_{J \rightarrow I}^{LS} \big/ A_{J \rightarrow I}^{BLSJ} \right) \omega_J^{LS}, \qquad 3.10.4$$

where,

$$A_{J \rightarrow I}^{BLSJ} = \sum_{i \in I} \sum_{j \in J} A_{j \rightarrow i}\, \omega_j^{Jo} \big/ \omega_J^{BLSJ} \qquad 3.10.5$$

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

$$\omega_J^{BLSJ} = \sum_{j \in J} \omega_j^{Jo} \qquad 3.10.6$$

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

$$Y(^{2S+1}L_J, {}^{2S'+1}L'_{J'}) = \sum_J \sum_{J'} \left(\frac{2J+1}{(2L+1)(2S+1)} \right) \left(\frac{2J'+1}{(2L'+1)(2S'+1)} \right) Y(^{2S+1}L, {}^{2S'+1}L') \qquad 3.10.7$$

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.

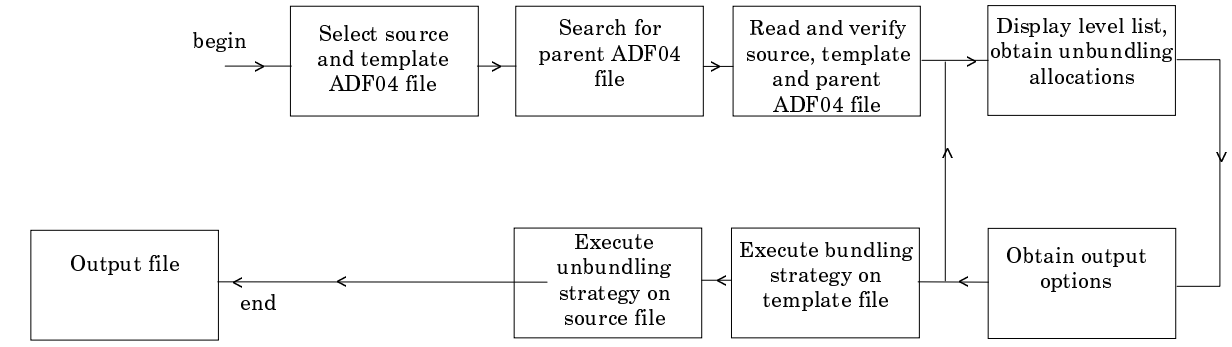
In unbundling, an additional template parent dataset at LSJ resolution is required and located by a search mechanism in ADAS210. If available, the parent configurations, parent energies and statistical weights are transcribed from the template following the selections entered by the user. Three types 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.

Program steps:

These are summarised in figure 3.10.

Figure 3.10



Interactive parameter comments:

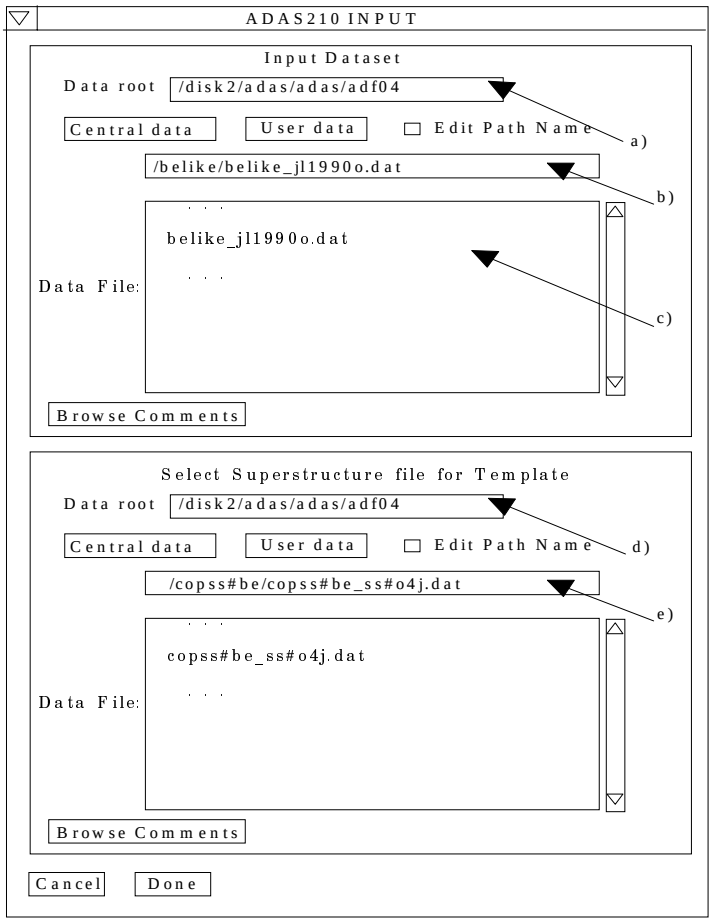
Programs of this series (ADAS2) which make use of data from archived ADAS datasets initiate an interactive dialogue with the user in three parts, namely, input file selection, entry of user data and disposition of output.

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. 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.

7. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.

8. 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.

9. 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*.

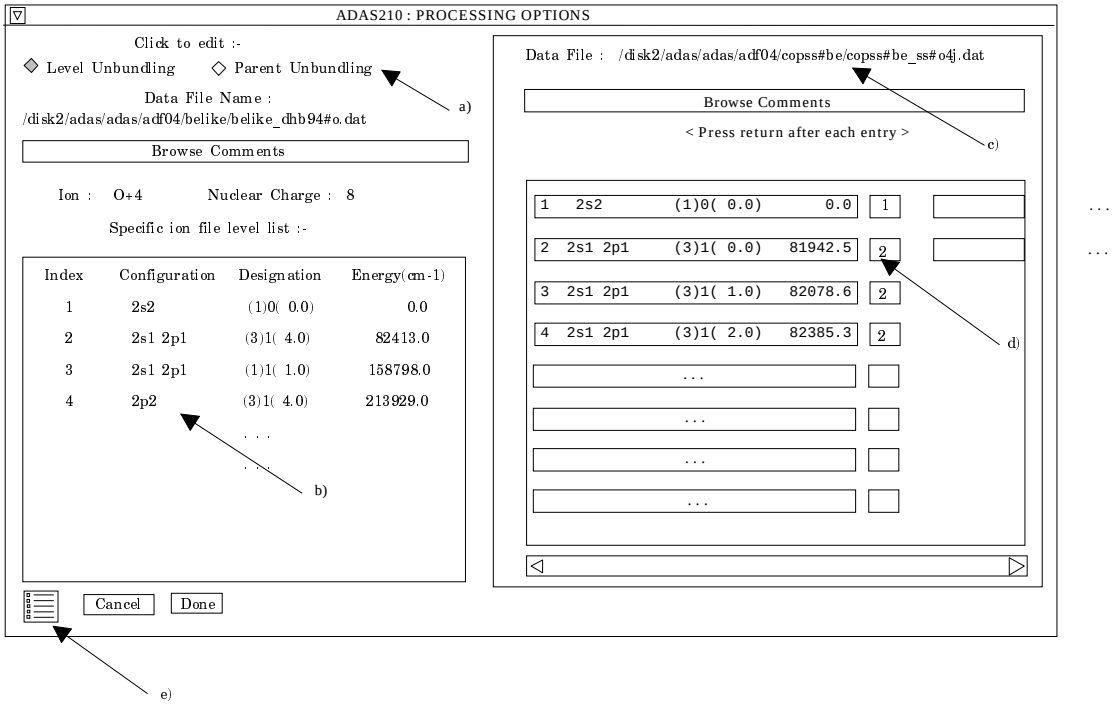
10. Once the data files are selected, the set of buttons at the bottom of the main window become active.

11. 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.

12. 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*).

13. 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



14. 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. Click the appropriate button to fill the left side level display window b) and the right side Unbundling window d).

15. 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.

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

17. 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. Ensure that no index numbers are omitted when entering them at d). 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**.

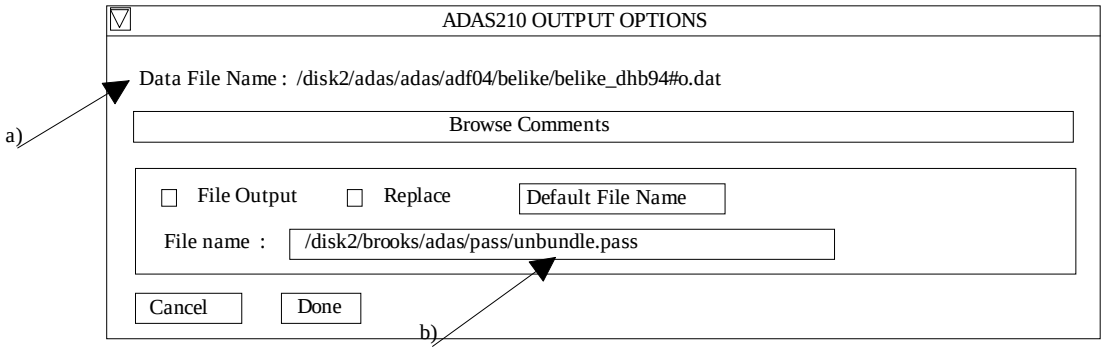
18. When you have finished the level allocation, click the *Parent Unbundling* button at a) to execute parent bundling. Note you may proceed to the next screen directly by clicking the *Done* button after level unbundling, but in this case a default '(1S)' parent is introduced. In this circumstance it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

19. 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.

20. 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. For basic studies, these issues may be ignored.

21. 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.



22. 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.

23. 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.

24. There is no graphical output option.

Illustration:

An example of a source data set for unbundling is given in table 3.10a and the unbundled output ADF04 file in table 3.10b. 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 3.10a

```
O + 4         8         5        918657.0(2S)
    1 2S2(1S0)          (1)0( 0.0)        0.0         {1}2.000
    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}2.000
    5 2P2(1D2)          (1)2( 2.0)   231721.4         {1}2.000
    6 2P2(1S0)          (1)0( 0.0)   287910.3         {1}2.000
    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
R  1  +1         2.83-13 2.01-13 1.22-13 8.20-14 5.61-14 3.86-14 2.99-14 1.88-14
R  2  +1         1.82-12 1.30-12 7.37-13 4.50-13 2.72-13 1.49-13 1.60-13 1.33-13
R  3  +1         4.36-13 3.12-13 1.80-13 1.13-13 6.95-14 3.71-14 3.09-14 2.31-14
R  4  +1         4.78-13 4.06-13 2.07-13 9.66-14 3.96-14 1.17-14 5.92-15 3.39-15
R  5  +1         5.24-13 4.73-13 2.49-13 1.17-13 4.82-14 1.34-14 5.00-15 1.90-15
R  6  +1         1.26-13 1.14-13 6.05-14 2.85-14 1.17-14 3.26-15 1.22-15 4.59-16
R  7  +1         9.38-14 6.84-14 5.68-14 5.52-14 4.67-14 2.59-14 1.56-14 8.97-15
R  8  +1         2.89-14 2.09-14 1.53-14 1.33-14 1.10-14 6.66-15 5.49-15 4.11-15
R  9  +1         1.27-13 8.93-14 5.46-14 3.70-14 2.38-14 1.58-14 2.20-14 2.19-14
R 10  +1         3.78-13 2.65-13 1.71-13 1.27-13 8.40-14 4.79-14 4.71-14 4.18-14
R 11  +1         4.47-13 2.99-13 2.06-13 1.87-13 1.30-13 5.97-14 4.47-14 3.45-14
R 12  +1         1.13-13 7.50-14 4.10-14 2.53-14 1.46-14 1.14-14 2.55-14 2.86-14
  -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-------------------------------------------------------------------------------
C  The radiative and dielectronic data is transcribed from
C  jetshp.belike.data(wjd92#o) which uses the same level set and
C  temperatures as the present dataset.  The comments from that
C  data set are repeated here.
C
C                                                 H.P.Summers 10.01.95
C-------------------------------------------------------------------------------
```

```
C  Radiative recombination data added - processed by adasrrc on
C                                       JETSHP.RADREC.BELIKE(O5LS)
C
C  H P Summers   Aug 1992.
C
C-----------------------------------------------------------------------
C
C     Dielectronic data is post-processed from Badnell files as follows:
C
C          /JETSHP.BADNELL.LILIKE(O5LS12)
C          /JETSHP.BADNELL.LILIKE(O5LS22)
C          /JETSHP.BADNELL.LILIKE(O5LS23)
C
C     The cross-referencing file is as follows:
C
C          /JETSHP.BADNELL.XREFDAT(O4L)
C
C     The parent metastable indices are as follows:
C
C     1.    1S2 2S1             (2)0( 0.5)
C
C     Dielectronic data added to  14 existing rad. recom. level sets
C
C                                          18/08/92
C-----------------------------------------------------------------------
```

Table 3.10b

```
O + 4         8         5   918657.0(2S)
    1 2S2(1S0)          (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 2S2P(1P1)         (1)1( 1.0)   158797.7
    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(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 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 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 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
   6   1 1.00-30 1.04-03 1.20-03 1.33-03 1.29-03 1.10-03 7.60-04 5.17-04 3.28-04
   7   1 1.00-30 3.11-03 3.60-03 4.00-03 3.87-03 3.31-03 2.28-03 1.55-03 9.83-04
   8   1 1.00-30 5.18-03 6.00-03 6.67-03 6.44-03 5.51-03 3.80-03 2.58-03 1.64-03
               . . .
               . . .
  17  15 1.25-30 4.37+00 4.74+00 6.72+00 8.82+00 1.10+01 1.34+01 1.47+01 1.57+01
  17  16 8.25-32 2.92-01 3.17-01 4.49-01 5.89-01 7.34-01 8.96-01 9.84-01 1.05+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: /packages/adas/adas/adf04/belike/belike_dhb94#o.dat
C  Template file:
C  /packages/adas/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    31   32   33   34   35   36   37   38   39   40
C    41   42   43   44   45   46
C  Source File Assignment:
C     1    1    1    1    1    1    1    1    1    1
C     2    2    2    2    2    2    2    2    2    2
C     3    4    5    6    7    8    9   10   11   12
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  Producer:  Stuart Loch
C  Date: 11/03/99
C
C--------------------------------------------------------------------------------
```

Notes: