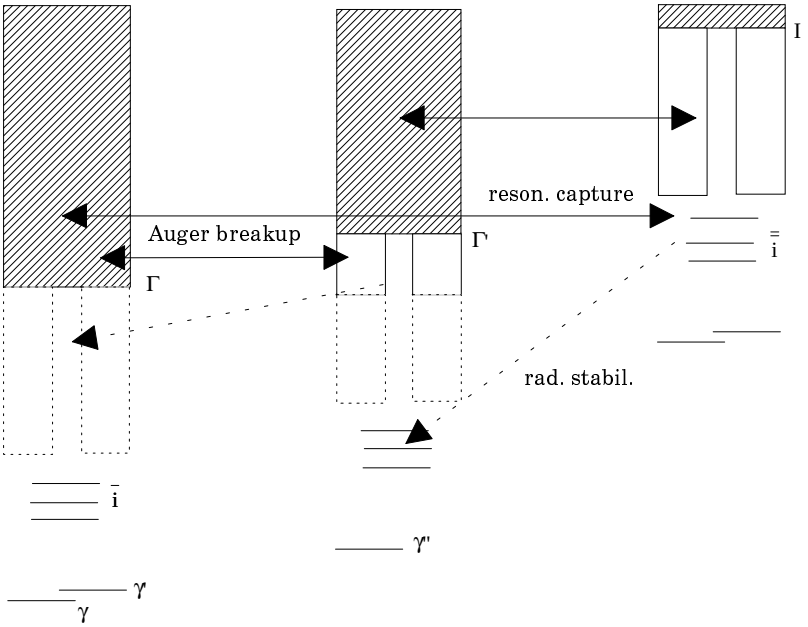
ADAS212: Dielectronic recombination - process for specific ion file

The program adds state selective dielectronic recombination coefficient data to specific ion files of type *adf04*. To achieve this it, it opens the primary data archives for dielectronic recombination coefficient data of type *adf09* and accesses the part of the data concerned with LS coupled low levels. The mapping of the data into the *adf04* files makes use of a cross-referencing file which must be set up prior to execution. Such cross-referencing files are archived in data format *adf18* and the particular sub-library of relevance here is *a09_a04*. The result of the operation of the code is a fully specified *adf04* file ready for immediate inclusion in your personal database.

Background theory:

The code and background theory is being extended to include the new intermediate coupling dielectronic data and *adf04* files at J-resolution. The following notes are incomplete.

Consider the recombination reaction for $z+1$ times ionised ion $\mathcal{A}^{+z+1}$ in the state Γ leaving a z times ionised ion $\mathcal{A}^{+z}$ in state i , Let the states i be partitioned into true bound states $\bar{i}$ and auto-ionising states $\overline{\overline{i}}$ and that the auto-ionising states of the ion $\mathcal{A}^{+z}$ are the set of terms $\{S_{\overline{\overline{i}}} L_{\overline{\overline{i}}} : \overline{\overline{i}} = 1,\ldots, N_z\}$. These are the intermediate states of the dielectronic recombination process. Let the ion $\mathcal{A}^{+z}$ have ground and metastable terms denoted by $\{S_\gamma L_\gamma : \gamma = 1,\ldots, M_z\}$. Also let the terms of the parent ion $\mathcal{A}^{+z+1}$ be the set $\{S_I L_I : I = 1,\ldots, N_{z+1}\}$ of which the subset $\{S_\Gamma L_\Gamma : \Gamma = 1,\ldots, M_{z+1}\}$ constitutes the metastables. We use small letters for recombined ion term indices and capital letters for recombining ion term indices. The improvement of ionisation data linking the metastables is the main concern. We seek to map relevant collision data from state selective dielectronic recombination rate coefficient archives of type *adf09* onto a specific ion file of type *adf04*.



The general specification of the *adf09* file includes parent states distinguishing those which are metastable and so can act as initial target states for the process. Final states are separated into individual resolved lower lying terms and then higher nl and n shells distinguished by spin system and parent upon which they are built. For the objectives of generalised collisional-radiative modelling, final states include those which are built on metastable parents although those can undergo further Auger breakup. Dielectronic recombination coefficients tabulated as a function of electron temperature are available for each initial and final state under these

classes. Additionally, for completeness, averaged Auger rates are available for n-shells built on metastables to lower parent metastables. The range of bundled n-shells is spanned by a representative set of n-shells. The mappings implemented by ADAS212 are only concerned with the individually labelled terms.

In general the mapping from *adf09* to *adf04* requires an alteration of the temperatures at which the data are stored in the *adf09* file to those required in the *adf04* file by interpolation. The known energies of the terms assist in providing accurate interpolation and such data are available in both files. It is convenient to indicate values relating to the *adf04* file by the superscript $^{\{04\}}$ and to the *adf09* file by the superscript $^{\{09\}}$. Thus the electron temperature set for the *adf04* file is $\{T_k^{\{04\}} : k = 1,\ldots, N_T^{\{04\}}\}$.

Since *adf04* files and *adf09* files are prepared independently (often exploiting different atomic structure codes) there is no certainty that the indexing of terms for the same ion in two such data sets will be the same. Also choice and indexing of metastables is to a degree at the choice of the user and varies with physical scenario. Thus it is necessary to match terms between the two file types with a cross-referencing file which is set up explicitly by hand. Cross-referencing files for the present purpose are archived in ADAS data format a*df18/a09_a04*.

Formally, *adf04* files and *adf09* files make almost no distinction between term and level resolution. The J-quantum number in level resolution data sets is written and handled as the (statistical weight-1)/2. It is only in the leading line of the *adf04* file (where a classification string for parents is written) that any difference occurs. Thus the above discussion applies equally to J-resolved level resolution. The cross-referencing file is where term/level distinction is made and steering of cross-transcription (term ---> level) may be set up.

The *adf09* tabulation is of the rate coefficient $\alpha_{\Gamma\to i}^{\{23\}}(T)$. The rate coefficient is strongly varying with temperature at low temperatures and may be zero for sufficiently low temperatures at machine precision in numerical tabulations. Let rate coefficients be zero at temperatures up to index number k_0. The code computes the quantities $\{F_{\Gamma\to i}^{\{09\}}(T_k^{\{09\}}): k = 1, N_T^{\{00\}}\}$ with $F_{\Gamma\to i}^{\{09\}}(T_k^{\{09\}}) = F_{\Gamma\to i}^{\{09\}}(T_{k_0+1}^{\{09\}})$ for $k = 1,\ldots, k_0$ and with

$$F_{\Gamma\to i}^{\{09\}}(T_k^{\{09\}}) = \exp(\Delta E_{i\Gamma}^{\{09\}})\alpha_{\Gamma\to i}^{\{09\}}(T_k^{\{09\}}) \qquad 3.12.1$$

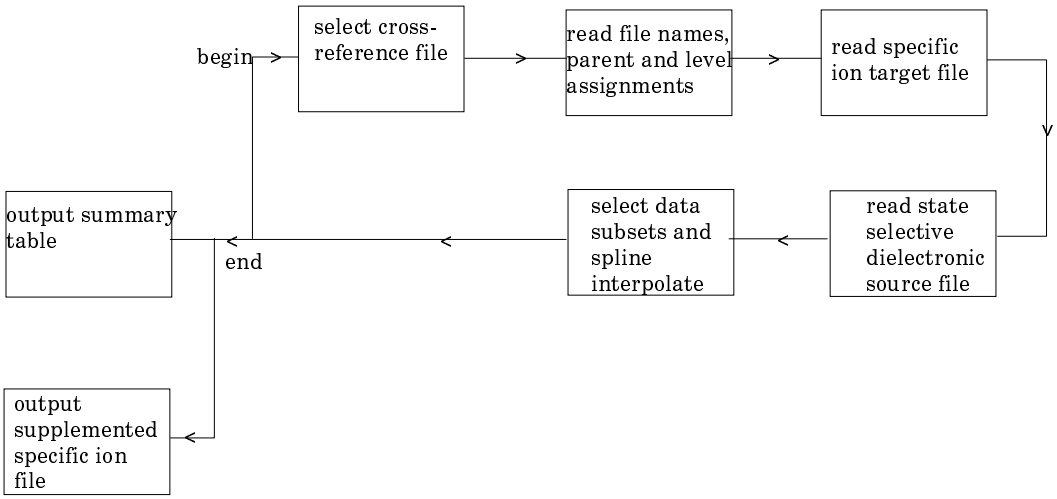
to regularise and smooth the rate coefficients. It is these latter forms which are interpolated in the log/log plane by cubic splines and then converted back to rate coefficients to provide data at the *adf04* file temperature set as $\{\alpha_{\Gamma\to i}^{\{04\}}(T_k^{\{04\}}): k = 1, N_T^{\{04\}}\}$. The spline is constructed to have zero gradient at the first node with zero gradient extrapolation and zero curvature at the last node with constant gradient extrapolation. As pointed out above, indexing of terms may not be identical in *adf04* and *adf09* files. A cross-reference table defines the one-to-one mapping $i^{\{04\}} \leftrightarrow i^{\{09\}}$.

Resolution detection and switching To be written.

Program steps:

These are summarised in figure 3.12.

Figure 3.12



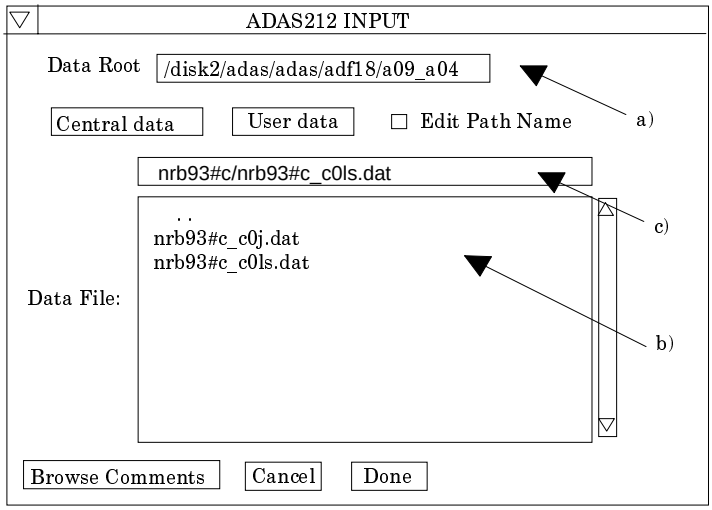
Interactive parameter comments:

Move to the directory in which you wish the output text file produced after executing any ADAS program (*paper.txt* is the default) to appear. There is no graphical output from this code. Initiate ADAS212 from the program selection menus in the usual manner.

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

1. An *adf18/a09_a04* format cross-referencing file is the appropriate input file for use by the program ADAS212. Your cross-referencing data should be held in such a file, in the same directory structure as central ADAS, but with your identifier replacing the first *adas.*

2. Available sub-directories are shown in the large file display window at b). Scroll bars appear if the number of entries exceed the file display window size. There are a large number of these. They are usually stored in sub-directories by isoelectronic sequence of the recombined ion with a prefix which identifies the primary author of the actual dielectronic data accessed. It is useful to use a naming convention for the final part of the file name which includes the ion and 'LS' (eg. nrb93#c/nrb93#c_c0ls.dat) to indicate that the data is for terms.



3. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then the individual datafiles are presented for selection. Datafiles all have the termination *.dat.*

4. Once a data file is selected, the set of buttons at the bottom of the main window become active.

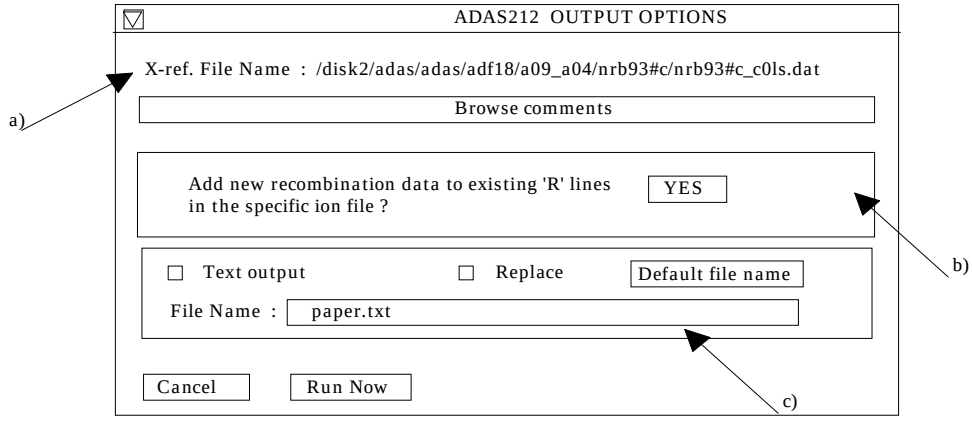
5. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what has gone into the dataset and the attribution of the dataset. The possibility of browsing the comments appears in the subsequent main window also.

6. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

There is no processing options window for ADAS212.

The **output options window** is shown below. There is no graphical output possibility but in addition to the usual text file, an output data file is always produced

7. The data output file is of specific ion file form, that is *adf04* and is sent to your pass directory as *adas213.pass*. It comprises the *adf04* file for which the cross-referencing was prepared but includes dielectronic data. It is the normal practice to use ADAS211 to put radiative recombination data in the specific ion file and then use ADAS212 to add the dielectronic data. The button at b) allows the choice of whether the dielectronic data should be added on to the radiative recombination 'R-lines' or replace them.



8. By pressing *Run Now* , you can wait for the output to be generated before continuing. When this option is taken a small information box opens showing the progress the program has made. Once this has been done the calculations cannot be halted, but an execution time of less than 30 seconds can usually be expected.

9. Since the code operates rapidly, we have removed the background execution operation available in the sister program ADAS211.

Illustration:

The following shows the supplementation of a helium-like file for carbon. Table 3.12a shows the cross-reference file of type adf18/a09_a04. The dielectronic data files are shown as the 'Badnell dielectronic files'. The cross-referencing shown in the list at the foot of the table maps from the dielectronic adf09 file indexing (bd1) to the specific ion file (sp). A section of the dielectronic adf09 file is shown in table 3.12d. Table 3.12b shows part of the adf04 file prior to supplementation and table 3.12c shows the supplemented file. Note that the dielectronic part is the 'R-lines'. Note also the addition to the comments describing the dielectronic data map at the foot of the comments section of the supplemented adf04 file.

Table 3.12a

```
Specific ion input file
------------------------
"ADASUSER"/adf04/helike/helike_wjd92#c.dat     : specific ion file for supplementation

Badnell dielectronic files
------------------------
"ADASCENT"/adf09/nrb93#h/nrb93#h_c5ls12.dat     : 1st. Badnell file of diel. data

Output files
------------------------
"ADASUSER"/pass/adas212_file2-12a.pass          : supplemented specific ion file
"ADASUSER"/pass/adas212_file2-12b.pass          : dielectronic data for MAINCL codes

Level cross-reference lists for specific ion and badnell files
---------------------------------------------------------------

    sp.        bd1.        bd2.        bd3.        bd4.        bd5.        bd6.
    ---        ----        ----        ----        ----        ----        ----
      1           0
```

```
      2          1
      3          2
      4          3
      5          4
      6          5
      7          7
      8          6
      9          8
     10          9
     11         10
```

Table 3.12b

```
C + 4         6         5       3162395.(2S)
    1   1S2             (1)0( 0.0)              0.    {1}2.00
    2   1S1 2S1         (3)0( 1.0)         2411262.    {1}1.00
    3   1S1 2S1         (1)0( 0.0)         2455024.    {1}1.00
    4   1S1 2P1         (3)1( 4.0)         2455225.    {1}1.00
    5   1S1 2P1         (1)1( 1.0)         2483371.    {1}1.00
    6   1S1 3S1         (3)0( 1.0)         2839562.    {1}1.00
    7   1S1 3S1         (1)0( 0.0)         2851180.    {1}1.00
    8   1S1 3P1         (3)1( 4.0)         2851418.    {1}1.00
    9   1S1 3D1         (3)2( 7.0)         2857310.    {1}1.00
   10   1S1 3D1         (1)2( 2.0)         2857529.    {1}1.00
   11   1S1 3P1         (1)1( 1.0)         2859375.    {1}1.00
   -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 4.86+01 3.01-02 2.80-02 1.89-02 1.47-02 1.14-02 8.17-03 6.32-03 4.34-03
   3   1 3.31+05 1.19-02 1.17-02 1.10-02 1.13-02 1.16-02 1.17-02 1.29-02 1.39-02
   4   1 9.55+06 4.70-02 4.51-02 3.85-02 3.75-02 3.50-02 2.92-02 2.36-02 1.71-02
   5   1 8.73+11 2.81-02 2.87-02 3.13-02 3.46-02 3.95-02 4.92-02 6.38-02 8.98-02

                          .        .        .

  10   9 1.00-30 1.07+01 7.14+00 4.12+00 2.89+00 2.07+00 1.45+00 1.12+00 7.06-01
  11   9 1.00-30 2.58+00 2.10+00 1.11+00 7.84-01 5.23-01 3.45-01 2.96-01 1.86-01
  11  10 4.36+04 7.05+01 6.77+01 4.77+01 4.83+01 5.34+01 6.32+01 6.89+01 7.62+01
  -1
  -1  -1
C-------------------------------------------------------------------------------
C
C  Energy levels
C  Taken from NSRDS NBS 3 Sect 3.
C
C  Ionisation potential
C  As energy levels.
C
C  A values
C  Taken from Tayal (Phys Rev A34, 1847, 1986)
C
C  Collision Data
C  Data taken from the same source as the A values. This paper was an
C  extension of earlier work by Tayal and Kingston (J Phys B 17, L145, 1984)
C  for the 1 1S - 2 3S and 1 1S - 2 3P transitions.  CI wavefunctions were
C  used for eleven target terms. Lower partial waves (l<=11) were calculated
C  by the R matrix method. For the higher partial waves, a close coupling
C  calculation with exchange omitted was done. Effective collision strengths
C  at eleven temperatures were tabulated. Theoretical energy levels were used
C  in JET excitation rate program.
C
C
C  J Lang    February 1990.
C
C  UPDATES:
C  --------
C
C  Forbidden A-values for 2-1, 3-1, 4-1 from Mcwhirter, Culham SS p265
C  added by WJD 11/6/91
C-------------------------------------------------------------------------------
```

Table 3.12c

```
C + 4         6         5       3162395.(2S)
    1   1S2             (1)0( 0.0)              0.    {1}2.00
    2   1S1 2S1         (3)0( 1.0)         2411262.    {1}1.00
    3   1S1 2S1         (1)0( 0.0)         2455024.    {1}1.00
    4   1S1 2P1         (3)1( 4.0)         2455225.    {1}1.00
    5   1S1 2P1         (1)1( 1.0)         2483371.    {1}1.00
    6   1S1 3S1         (3)0( 1.0)         2839562.    {1}1.00
    7   1S1 3S1         (1)0( 0.0)         2851180.    {1}1.00
    8   1S1 3P1         (3)1( 4.0)         2851418.    {1}1.00
    9   1S1 3D1         (3)2( 7.0)         2857310.    {1}1.00
   10   1S1 3D1         (1)2( 2.0)         2857529.    {1}1.00
   11   1S1 3P1         (1)1( 1.0)         2859375.    {1}1.00
   -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 4.86+01 3.01-02 2.80-02 1.89-02 1.47-02 1.14-02 8.17-03 6.32-03 4.34-03
   3   1 3.31+05 1.19-02 1.17-02 1.10-02 1.13-02 1.16-02 1.17-02 1.29-02 1.39-02
   4   1 9.55+06 4.70-02 4.51-02 3.85-02 3.75-02 3.50-02 2.92-02 2.36-02 1.71-02
   5   1 8.73+11 2.81-02 2.87-02 3.13-02 3.46-02 3.95-02 4.92-02 6.38-02 8.98-02

                          .        .        .
  10   9 1.00-30 1.07+01 7.14+00 4.12+00 2.89+00 2.07+00 1.45+00 1.12+00 7.06-01
  11   9 1.00-30 2.58+00 2.10+00 1.11+00 7.84-01 5.23-01 3.45-01 2.96-01 1.86-01
```

```
  11  10 4.36+04 7.05+01 6.77+01 4.77+01 4.83+01 5.34+01 6.32+01 6.89+01 7.62+01
R  1  +1         1.00-30 1.00-30 1.00-30 1.00-30 1.00-30 1.00-30 1.00-30 1.00-30
R  2  +1         1.00-30 8.90-38 2.78-22 2.28-17 3.93-15 4.16-14 5.14-14 3.41-14
R  3  +1         1.00-30 1.00-30 9.20-26 1.45-19 1.14-16 3.02-15 5.06-15 3.90-15
R  4  +1         1.00-30 3.39-39 3.84-23 4.84-18 1.03-15 1.22-14 1.57-14 1.06-14
R  5  +1         1.00-30 2.22-38 1.65-22 1.95-17 4.05-15 4.80-14 6.16-14 4.16-14
R  6  +1         1.00-30 1.00-30 7.22-25 9.36-19 6.34-16 1.49-14 2.39-14 1.80-14
R  7  +1         1.00-30 1.00-30 1.64-25 2.47-19 1.80-16 4.44-15 7.23-15 5.48-15
R  8  +1         1.00-30 1.00-30 3.67-25 5.28-19 3.77-16 9.19-15 1.49-14 1.13-14
R  9  +1         1.00-30 1.00-30 1.89-24 2.71-18 1.93-15 4.68-14 7.57-14 5.73-14
R 10  +1         1.00-30 1.00-30 8.09-25 1.35-18 1.03-15 2.62-14 4.31-14 3.29-14
R 11  +1         1.00-30 1.00-30 6.61-25 9.71-19 7.02-16 1.72-14 2.80-14 3.12-14
  -1
  -1  -1
C-------------------------------------------------------------------------------
C
C  Energy levels
C  Taken from NSRDS NBS 3 Sect 3.
C
C  Ionisation potential
C  As energy levels.
C
C  A values
C  Taken from Tayal (Phys Rev A34, 1847, 1986)
C
C  Collision Data
C  Data taken from the same source as the A values. This paper was an
C  extension of earlier work by Tayal and Kingston (J Phys B 17, L145, 1984)
C  for the 1 1S - 2 3S and 1 1S - 2 3P transitions.  CI wavefunctions were
C  used for eleven target terms. Lower partial waves (l<=11) were calculated
C  by the R matrix method. For the higher partial waves, a close coupling
C  calculation with exchange omitted was done. Effective collision strengths
C  at eleven temperatures were tabulated. Theoretical energy levels were used
C  in JET excitation rate program.
C
C
C  J Lang    February 1990.
C
C  UPDATES:
C  --------
C
C  Forbidden A-values for 2-1, 3-1, 4-1 from Mcwhirter, Culham SS p265
C  added by WJD 11/6/91
C-------------------------------------------------------------------------------
C
C     Dielectronic data is post-processed from Badnell files as follows:
C
C      /u/adas/adas/adf09/nrb93#h/nrb93#h_c5ls12.dat
C
C     The cross-referencing file is as follows:
C
C      /u/hps/adas/adf18/a09_a04/nrb93#he/nrb93#he_c4ls.dat
C
C     The parent metastable indices are as follows:
C
C     1.    1S1                (2)0( 0.5)
C
C     Dielectronic data added to   0 existing rad. recom. level sets
C
C                                            14/04/98
C-------------------------------------------------------------------------------
```

Table 3.12d

```
SEQ='HE'     NUCCHG= 6

  PARENT TERM INDEXING            BWNP=   3950474.0   NPRNTI= 1   NPRNTF= 1
  --------------------
  INDP    CODE                 S L   WI        WNP
  ----    ----                 - -   --  ----------
    1     1S1                 (2)0( 0.5)        0.0

  LS RESOLVED TERM INDEXING       BWNR=   4694405.8    NTRM= 58
  -------------------------
  INDX    CODE                 S L   WJ        WNR
  ----    ----                 - -   --  ----------
    1     1S1 2S1             (3)0( 1.0)        0.0
    2     1S1 2P1             (3)1( 4.0)    46802.2
    3     1S1 2S1             (1)0( 0.0)    51805.0
    4     1S1 2P1             (1)1( 1.0)    86592.9
    5     1S1 3S1             (3)0( 1.0)   421262.4
    6     1S1 3P1             (3)1( 4.0)   433333.9
    7     1S1 3S1             (1)0( 0.0)   434580.1
    8     1S1 3D1             (3)2( 7.0)   438943.7
    9     1S1 3D1             (1)2( 2.0)   439252.9
   10     1S1 3P1             (1)1( 1.0)   443967.6

                     .        .       .

   55     1S1 8G1             (1)4( 4.0)   697367.1
   56     1S1 8F1             (1)3( 3.0)   697367.5
   57     1S1 8D1             (1)2( 2.0)   697379.7
   58     1S1 8P1             (1)1( 1.0)   697548.6

  N-SHELL INDEXING & AUGER RATES                      NREP= 42
  ------------------------------
```

```
  IREP    N
  ----    -
    1     1
    2     2
    3     3

                     .       .       .

   39   535
   40   700
   41   811
   42   999



--------------------------------
PRTI= 1  TRMPRT= (2S)  SPNPRT= 2

  INDX TE=  2.50E+04  5.00E+04  1.25E+05  2.50E+05  5.00E+05  1.25E+06  2.50E+06  5.00E+06  1.25E+07  2.50E+07
  ---- ---
    1       0.00E+00  8.90E-38  2.78E-22  2.28E-17  3.93E-15  4.16E-14  5.14E-14  3.41E-14  1.26E-14  5.04E-15
    2       0.00E+00  0.00E+00  9.20E-26  1.45E-19  1.14E-16  3.02E-15  5.06E-15  3.90E-15  1.57E-15  6.50E-16
    3       0.00E+00  3.39E-39  3.84E-23  4.84E-18  1.03E-15  1.22E-14  1.57E-14  1.06E-14  3.94E-15  1.59E-15

                     .       .       .

   56       0.00E+00  0.00E+00  6.30E-27  4.43E-20  6.98E-17  2.73E-15  5.19E-15  4.25E-15  1.78E-15  7.45E-16
   57       0.00E+00  0.00E+00  2.53E-26  1.78E-19  2.81E-16  1.10E-14  2.09E-14  1.71E-14  7.18E-15  3.00E-15
   58       0.00E+00  0.00E+00  2.21E-26  1.55E-19  2.44E-16  9.54E-15  1.81E-14  1.48E-14  6.21E-15  2.60E-15


----------------------------------------
PRTF= 1  TRMPRT= (2S)  SPNPRT= 2  NSYS= 2
                                                                                                 -----------------
                                                                                                 SYS= 1  SPNSYS= 1
  IREP
  ----
    2       0.00E+00  2.56E-38  2.04E-22  2.43E-17  5.08E-15  6.02E-14  7.73E-14  5.22E-14  1.95E-14  7.84E-15
    3       0.00E+00  0.00E+00  1.63E-24  2.56E-18  1.92E-15  4.79E-14  7.84E-14  5.96E-14  2.39E-14  9.83E-15
    4       0.00E+00  0.00E+00  4.00E-25  1.35E-18  1.47E-15  4.61E-14  8.13E-14  6.42E-14  2.63E-14  1.09E-14

                     .       .       .

   40       0.00E+00  0.00E+00  2.40E-31  2.16E-24  3.85E-21  1.62E-19  3.16E-19  2.62E-19  1.10E-19  4.63E-20
   41       0.00E+00  0.00E+00  1.54E-31  1.39E-24  2.48E-21  1.04E-19  2.03E-19  1.68E-19  7.10E-20  2.98E-20
   42       0.00E+00  0.00E+00  8.26E-32  7.43E-25  1.32E-21  5.58E-20  1.09E-19  9.01E-20  3.80E-20  1.59E-20

                                                                                                 -----------------
                                                                                                 SYS= 2  SPNSYS= 3
  IREP
  ----
    2       0.00E+00  8.90E-38  2.78E-22  2.30E-17  4.04E-15  4.46E-14  5.65E-14  3.80E-14  1.42E-14  5.69E-15
    3       0.00E+00  0.00E+00  2.98E-24  4.17E-18  2.94E-15  7.09E-14  1.15E-13  8.66E-14  3.46E-14  1.42E-14

                     .       .       .

   39       0.00E+00  0.00E+00  1.14E-31  1.03E-24  1.83E-21  7.73E-20  1.50E-19  1.25E-19  5.26E-20  2.21E-20
   40       0.00E+00  0.00E+00  5.11E-32  4.59E-25  8.19E-22  3.45E-20  6.71E-20  5.57E-20  2.35E-20  9.85E-21
   41       0.00E+00  0.00E+00  3.28E-32  2.95E-25  5.27E-22  2.22E-20  4.32E-20  3.58E-20  1.51E-20  6.33E-21
   42       0.00E+00  0.00E+00  1.76E-32  1.58E-25  2.82E-22  1.19E-20  2.31E-20  1.92E-20  8.08E-21  3.39E-21
```

Notes: