

ADAS215: Specific ion file - temperature regrid

This is a new code which is not part of JET-ADAS. It alters the electron collisional rate coefficient (Upsilon) data in a specific ion file of format *adf04* to a different set of electron temperatures for which it creates a new specific ion file. Extrapolation may be attempted with the code and this is an indeterminate error amplifying process in general. The code seeks to minimise this by supporting interpolation and extrapolation with Burgess-Tully C-plots, selective display of scaled collision rate coefficients and control of Burgess-Tully types and C parameters.

Background theory:

ADAS specific ion files of type *adf04* store electron impact transition data in the form of ‘thermally averaged collision strengths’ or ‘rate parameters’, Y , defined by

$$Y_{ij} = \int_0^{\infty} \Omega_{ij} e^{-E_j/kT_e} d(E_j / kT_e) \quad 3.15.1$$

for a collisional transition between states i and j with Ω_{ij} the collision strength, E_j the colliding electron energy after excitation has occurred and T_e the electron temperature. Let E_{ij} be the transition energy.

Burgess & Tully (1992) examined the behaviour of Y as a function T_e , and defined reduced variables appropriately so that the whole variation of Y and T_e could be mapped onto a finite range. They introduced a reduced temperature, x , and reduced Upsilon, y , for four types of transition. These are given below together with their limiting values when known. Burgess & Tully vary the parameter C to balance the spread of x -values across the range [0,1] and so optimise a five point, fixed knot, least squares spline through the data. This gives a compact representation of the data and a good control or check of the limiting high energy behaviour of the rate coefficient.

Type 1 - dipole:

$$x = 1 - \frac{\ln C}{\ln \left(\frac{kT_e}{E_{ij}} + C \right)} \quad 3.15.2$$

$$y(x) = \frac{Y}{\ln \left(\frac{kT_e}{E_{ij}} + e \right)} \quad 3.15.3$$

$$\text{with } y(0) = \Omega(0), \quad y(1) = \frac{4\omega_i f_{i \rightarrow j}}{E_{ij}}$$

Type 2 - non-dipole, non-spin change:

$$x = \frac{\left(\frac{kT_e}{E_{ij}} \right)}{\left(\frac{kT_e}{E_{ij}} + C \right)} \quad 3.15.4$$

$$y(x) = Y \quad 3.15.5$$

with $y(0) = \Omega(0)$, $y(1) = \text{high energy Born limit of } \Omega$.

Type 3 - spin change:

$$x = \frac{\left(\frac{kT_e}{E_{ij}}\right)}{\left(\frac{kT_e}{E_{ij}} + C\right)} \quad 3.15.6$$

$$y(x) = \left(\frac{kT_e}{E_{ij}} + 1\right)Y \quad 3.15.7$$

$$\text{with } y(0) = \Omega(0), \quad y(1) = \int_0^{\infty} \Omega d\left(\frac{E_j}{E_{ij}}\right).$$

Type 4 - weak oscillator strength:

$$x = 1 - \frac{\ln C}{\ln\left(\frac{kT_e}{E_{ij}} + C\right)} \quad 3.15.8$$

$$y(x) = \frac{Y}{\ln\left(\frac{kT_e}{E_{ij}} + C\right)} \quad 3.15.9$$

$$\text{with } y(0) = \frac{\Omega(0)}{\ln C}, \quad y(1) = \text{as for type 1.}$$

For the present code, the Burgess & Tully transformations are used as an aid to interpolation and extrapolation. That is an interpolating spline rather than a least squares optimising spline is passed through the Upsilon data for a transition. The collision data from the *adf04* file does not in general have all the information ideally required for assigning to type and to specify threshold and high energy limits. For an LS-coupled data set, the total spin quantum numbers are available and so assignment to type 3 is possible. For intermediate coupling data sets, this is less clear and the categorisation has to be supported by the manifest decreasing behaviour of Upsilon at high temperature. Since the *adf04* file includes the A-value for the transition, identification of type 1 and separation from type 2 is possible. The switch from type 1 to type 4 and from type 3 to type 4 is less clear and somewhat subjective.

It is to be noted that the first column of the *adf04* file electron impact transition lines contains a code for type assignment (1,2,3 or 4) although in virtually all data sets this is left blank. This indicates an unspecified type and the interpolating codes simply make a best guess according to the data and quantum numbers of the levels presented.

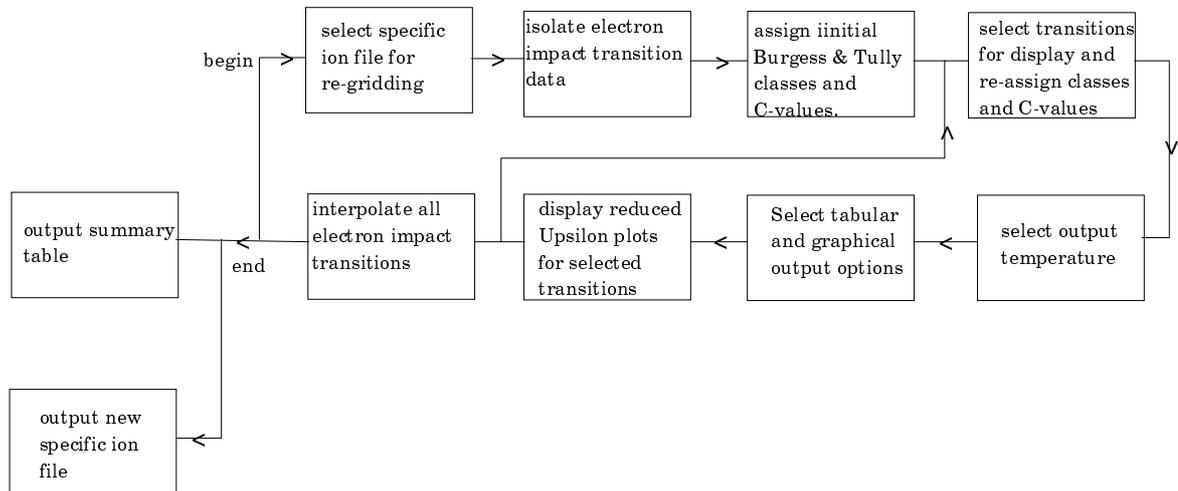
The main danger of the above automatic procedures is in extrapolation. It is desirable that a graph of uncertain cases should be presented and some capability to steer the interpolation/extrapolation be introduced. ADAS215 does this by allowing a selection of transitions to be displayed and allowing the *C* parameter and type for these to be assigned. For all other transitions a default setting for the *C* parameter is used and the type is determined automatically by the code. Where threshold and high temperature limits are not specified, the interpolating spline is designed to have zero curvature at its end points and extrapolation is by a straight line at the end point gradient.

Improvement to the interpolation/extrapolation can therefore be made by cycling repeatedly through the code. It should be noted that most *adf04* files have a temperature range which more than covers all physically relevant conditions and so some judgement is required as to how much effort is warranted in the re-gridding.

Program steps:

These are summarised in figure 3.15

Figure 3.15

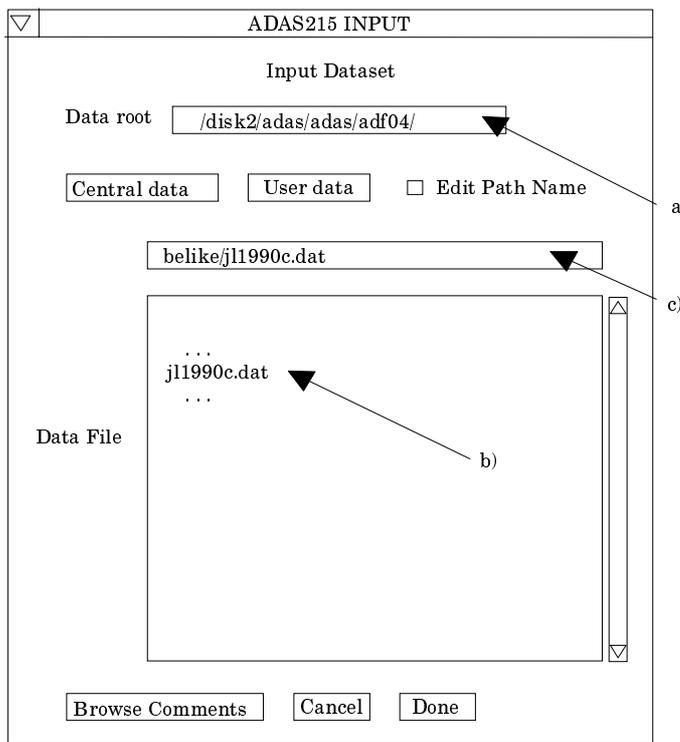


Interactive parameter comments:

Move to the sub-directory in which you wish graphic or text output from this program to appear. Initiate ADAS215 from the program selection menus in the usual manner.

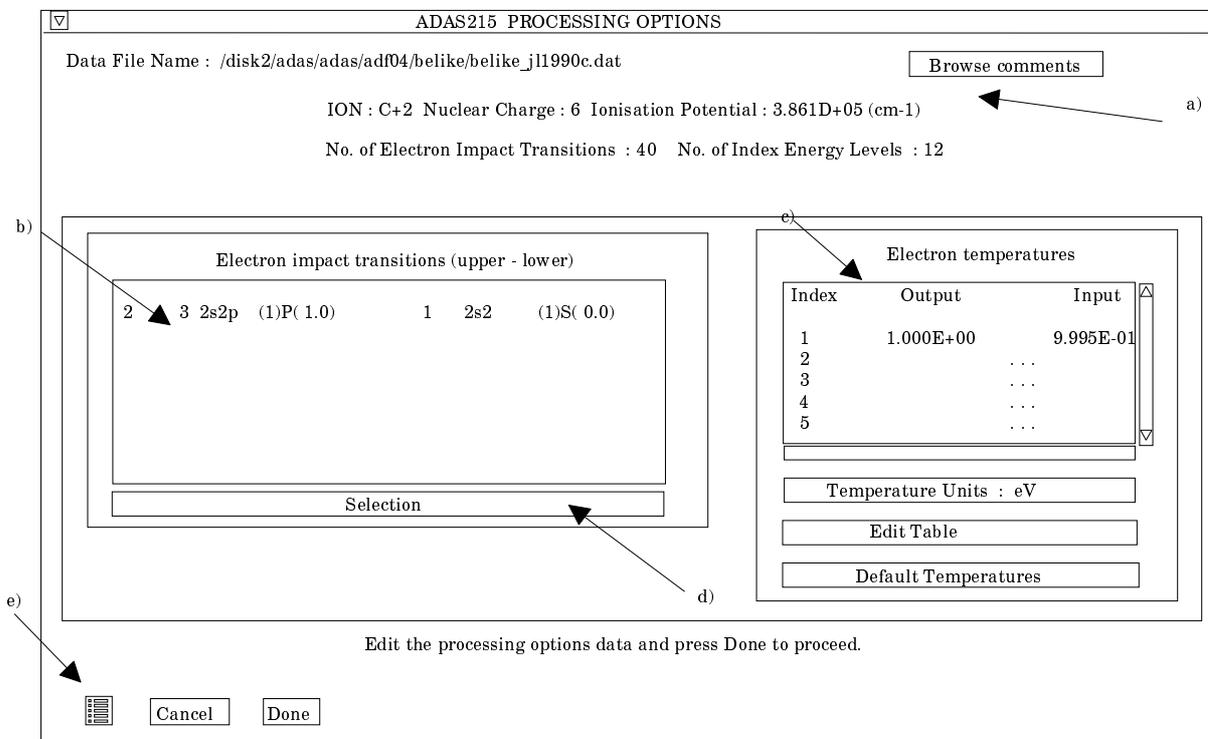
The **file selection window** has the appearance shown below

1. Data root a) shows the full pathway to the appropriate data sub-directories. 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 data files are presented for selection. Data files 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 data file. It is important to use this facility to find out what is broadly available in the data set. 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

- An arbitrary title may be given for the case being processed. For information the full pathway to the *adf04* file selected for temperature re-gridding is also shown. The button *Browse comments* a) allows display of the information field section at the foot of the selected *adf04*, if it exists.



- The sub-window at c) shows the *Input* temperatures from the *adf04* file and the *Output* temperatures at which the new *adf04* file is to be produced. Click on the *Edit Table* button to change the output values. Click on the *Default Temperatures* button to insert the default output temperature set. Note that the default set of temperatures is the standard 'z-scaled' set used for iso-electronic sequences preparation since 1997.

18. Hard copy is activated by the *Enable Hard Copy* button c). The File name box then becomes editable. If the output graphic file already exists and the *Replace* button has not been activated, a 'pop-up' window issues a warning.
19. A choice of output graph plotting devices is given in the Device list window. Clicking on the required device selects it. It appears in the selection window above the Device list window.
20. At d) the *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name 'paper.txt' may be set by pressing the button *Default file name*. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated.
21. At e) output of the re-gridded *adf04* file may be enabled. The *Default file* is set up at the first pass through this window. Note that the actual output is deferred. This is to allow further adjustment of rate coefficient interpolations before the final complete *adf04* is written. The re-gridded *adf04* file is placed by default in your */pass* directory as *adas215_adf04.pass*.
22. **N.B. In the re-gridded *adf04* file all transition lines other than electron impact transitions between bound states are deleted.** That is 'R-lines', 'S-lines', 'H-lines', 'P-lines' and 'I-lines'. Interpolation /extrapolation for these categories is much less secure than recreating the data for the new temperature grid as described in the following sections. Temperature re-gridding should be done as the first step in the chain of processing.
23. The graph is displayed in a following Graphical Output window.
24. At the base of the window, the icon for *Exit to Menu* is present. 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.

Illustration:

Figure 3.15a

UPSILON INTERPOLATION VS TEMPERATURE

ADAS : ADAS RELEASE: ADAS98 V2.1 PROGRAM: ADAS215 V1.1 DATE: 16/03/99 TIME: 16:10
 FILE : /disk3/summers/adas/adf04/cop98#10/belike_jl98#ne6j.dat
 KEY : (DASH LINE - INPUT DATA) (CROSSES - INTERPOLATION)

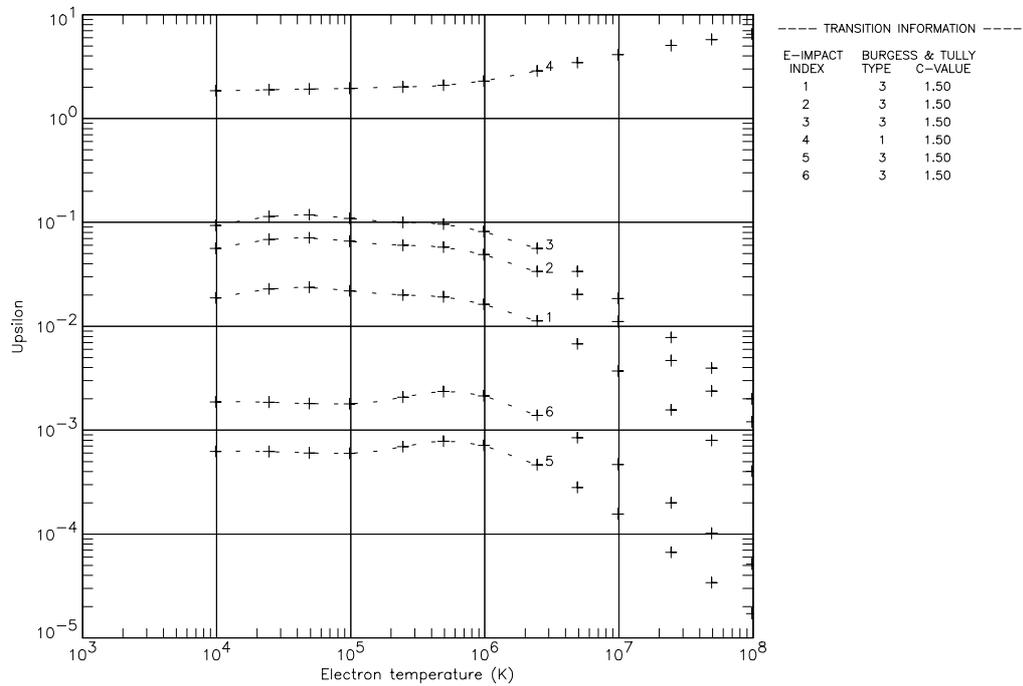


Table 3.15a

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ADAS RELEASE: ADAS98 V2.1 PROGRAM: ADAS215 V1.1 DATE: 16/03/99 TIME: 16:10
***** TABULAR OUTPUT FROM TEMPERATURE REGRIDDING PROGRAM: ADAS215 - DATE: 16/03/99 *****

INPUT ADF04 FILE NAME : /disk3/summers/adas/adf04/cop98#10/belike_jl98#ne6j.dat

ION      NUCLEAR      RECOMBINING      ----- IONIZATION POTENTIAL -----
CHARGE (Z0)      ION CHARGE (Z1)      (wave number <cm-1>)      (rydbergs)
-----
NE+ 6      10      7      1671792.      15.2345222

----- ENERGY LEVELS -----
INDEX  CONFIGURATION      (2S+1)L(J) - ENERGY RELATIVE TO LEVEL 1 - ENERGY RELATIVE TO IONISATION POTENTIAL
      (wave number <cm-1>)      (rydbergs)      (wave number <cm-1>)      (rydbergs)
-----
1  2s2      (1)0( 0.0)      0.      0.0000000      1671792.      15.2345222
2  2S1 2P1      (3)1( 0.0)      111254.      1.0138232      1560538.      14.2206990
3  2S1 2P1      (3)1( 1.0)      111708.      1.0179604      1560084.      14.2165619
. . .
45 2P1 3D1      (1)3( 3.0)      1214120.      11.0638992      457672.      4.1706231
46 2P1 3D1      (1)1( 1.0)      1219390.      11.1119231      452402.      4.1225992

-- INPUT ADF04 FILE TEMPERATURES: (TE=TP=TH) --
INDEX      (kelvin)      (eV)      (reduced)
-----
1      1.00D+04      8.62D-01      2.04D+02
2      1.58D+04      1.36D+00      3.22D+02
3      2.51D+04      2.16D+00      5.12D+02
4      3.98D+04      3.43D+00      8.12D+02
5      6.31D+04      5.44D+00      1.29D+03
6      1.00D+05      8.62D+00      2.04D+03
7      1.58D+05      1.36D+01      3.22D+03
8      2.51D+05      2.16D+01      5.12D+03
9      3.98D+05      3.43D+01      8.12D+03
10     6.31D+05      5.44D+01      1.29D+04
11     1.00D+06      8.62D+01      2.04D+04
12     2.51D+06      2.16D+02      5.12D+04

INPUT ADF04 FILE INFORMATION:
  
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-----
NUMBER OF ELECTRON IMPACT TRANSITIONS = 405
NUMBER OF PROTON IMPACT TRANSITIONS = 0
NUMBER OF CHARGE EXCHANGE RECOMBINATIONS = 0
NUMBER OF FREE ELECTRON RECOMBINATIONS = 0

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-- OUTPUT ADF04 FILE TEMPERATURES: (TE=TP=TH) --
INDEX      (kelvin)      (eV)      (reduced)
-----
 1      9.80D+03      8.44D-01      2.00D+02
 2      2.45D+04      2.11D+00      5.00D+02
 3      4.90D+04      4.22D+00      1.00D+03
 4      9.80D+04      8.44D+00      2.00D+03
 5      2.45D+05      2.11D+01      5.00D+03
 6      4.90D+05      4.22D+01      1.00D+04
 7      9.80D+05      8.44D+01      2.00D+04
 8      2.45D+06      2.11D+02      5.00D+04
 9      4.90D+06      4.22D+02      1.00D+05
10      9.80D+06      8.44D+02      2.00D+05
11      2.45D+07      2.11D+03      5.00D+05
12      4.90D+07      4.22D+03      1.00D+06
13      9.80D+07      8.44D+03      2.00D+06

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-- OUTPUT ADF04 FILE INTERPOLATION PARAMETERS --
IND  IU - IL  T  C-VAL  IND  IU - IL  T  C-VAL  IND  IU - IL  T  C-VAL  IND  IU - IL  T  C-VAL
-----
 1   2 - 1  3  1.500   2   3 - 1  3  1.500   3   4 - 1  3  1.500   4   5 - 1  1  1.500
 5   6 - 1  3  1.500   6   7 - 1  3  1.500   7   8 - 1  3  1.500   8   9 - 1  2  1.500
 9  10 - 1  2  1.500  10  11 - 1  3  1.500  11  12 - 1  2  1.500  12  13 - 1  1  1.500

401 42 - 10 3  1.500 402 43 - 10 3  1.500 403 44 - 10 2  1.500 404 45 - 10 2  1.500
405 46 - 10 1  1.500 406  0 -  0  `  0.000 407  0 -  0  `  0.000 408  0 -  0  `  0.000

```

Table 3.15b

```

NE+ 6      10      7      1671792.(1S)
 1 2s2      (1)0( 0.0)      0.0      {1}1.000
 2 2S1 2P1      (3)1( 0.0)      111254.0      {1}1.000
 3 2S1 2P1      (3)1( 1.0)      111708.0      {1}1.000

 45 2P1 3D1      (1)3( 3.0)      1214120.0      {1}1.000
 46 2P1 3D1      (1)1( 1.0)      1219390.0      {1}1.000
-1
7.00  3      9.80+03 2.45+04 4.90+04 9.80+04 2.45+05 4.90+05 9.80+05 2.45+06 4.90+06 9.80+06 2.45+07
 2  1 1.00-30 1.87-02 2.29-02 2.36-02 2.20-02 2.00-02 1.92-02 1.63-02 1.13-02 6.78-03 3.71-03 1.57-03
 3  1 1.86+04 5.61-02 6.86-02 7.08-02 6.59-02 6.01-02 5.76-02 4.89-02 3.37-02 2.03-02 1.11-02 4.67-03

 45 10 1.00-30 1.30-02 1.09-02 1.01-02 9.91-03 1.05-02 1.18-02 1.35-02 1.28-02 1.16-02 1.07-02 1.00-02
 46 10 1.72+11 4.28-01 3.68-01 3.62-01 3.75-01 4.08-01 4.58-01 5.43-01 6.85-01 8.42-01 1.05+00 1.38+00
-1
-1 -1
C-----
C
C File generated by altering the temperature set of an ADF04 file
C
C Program: ADAS215
C
C Source file: /disk3/summers/adas/adf04/cop98#10/belike_jl98#ne6j.dat
C
C Producer: summers
C
C Date: 16/03/99
C-----

```

Notes: