ADAS410: Dielectronic recombination – graph and fit data

The code allows interrogation of state selective dielectronic recombination data of ADAS data format *adf09*. The ADAS data base now contains very large collections of such data spanning all the ions of elements up to neon. *adf09* includes state selective dielectronic data to resolved lower lying LS-coupled (*ls*) terms or intermediate coupled (*ic*) J-levels, dielectronic data to representative n-shells (*ls* case) or nl-shells (*ic* case) separated according to parents and spin systems and averaged Auger data. All of these data can be extracted and displayed by the code.

Background theory:

The code and background theory is being extended to include the new intermediate coupling dielectronic data. The following notes are incomplete.

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 $\mathscr{A}^{+z+1}$ in the state Γ leaving a z times ionised ion $\mathscr{A}^{+z}$ 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 $\mathscr{A}^{+z}$ are the set of terms $\{S_i L_i : \overline{\overline{i}} = 1, \dots, N_z\}$ in the *ls* case or the set of levels $\{S_i L_i J_i : \overline{\overline{i}} = 1, \dots, N_z\}$ in the *ic* case. These are the intermediate states of the dielectronic recombination process. Let the ion $\mathscr{A}^{+z}$ have ground and metastable terms denoted by $\{S_\gamma L_\gamma : \gamma = 1, \dots, M_z\}$ in the *ls* case or $\{S_\gamma L_\gamma J_\gamma : \gamma = 1, \dots, M_z\}$ in the *ic* case. Also let the terms or levels of the parent ion $\mathscr{A}^{+z+1}$ be the set $\{S_I L_I : I = 1, \dots, N_{z+1}\}$ or $\{S_I L_I J_I : I = 1, \dots, N_{z+1}\}$ with the subset $\{S_\Gamma L_\Gamma : \Gamma = 1, \dots, M_{z+1}\}$ or $\{S_\Gamma L_\Gamma J_\Gamma : \Gamma = 1, \dots, M_{z+1}\}$ constituting the metastables in the *ls* or *ic* cases respectively. We use small letters for recombined ion term indices and capital letters for recombining ion term indices.
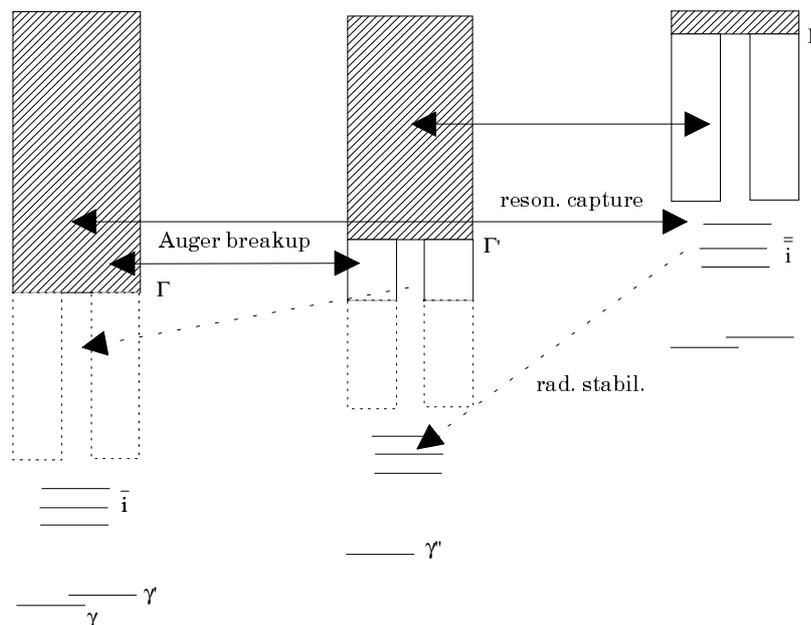
The general specification of the *adf09* file includes parent states distinguishing those which are metastable and so can act as initial target states for the process. Final states are separated into individual resolved lower lying terms and then higher n shells distinguished by spin system and parent upon which they are built in the *ls* case. In the *ic* case, 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 $\{T_k^{\{04\}} : k = 1, ..., N_T^{\{04\}}\}$.

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 $k = 1, ..., k_0$ and with

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

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 5.10.

Figure 5.10

```
                    ┌──────────────┐          ┌──────────────┐          ┌──────────────┐
                    │ select adf09 │          │ read and sort│          │input user data│
        begin ────► │ dielectronic │ ───────► │ complete data│ ───────► │ sub-selection│
                    │ file         │          │ from file    │          │ and ouput    │
                    └──────────────┘          └──────────────┘          │ temperatures │
                                                                         └──────────────┘

    ┌──────────────┐          ┌──────────────┐          ┌──────────────┐
    │output summary│          │ Display rate │          │ spline       │
    │table and     │ ◄─────── │ coefficient  │ ◄─────── │ interpolate  │
    │graphs        │   end    │ graph        │          │ to user      │
    └──────────────┘          └──────────────┘          │ temperatures │
                                                         └──────────────┘
```
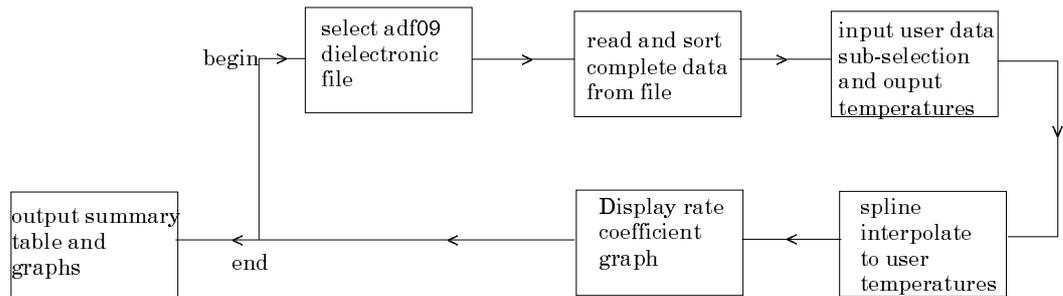
Interactive parameter comments:

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

1. Data root a) shows the full pathway to the appropriate data subdirectories of type *adf09*. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. 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*. Note the notation used for dielectronic data file names, that is, *<ion>ls<nn'>* with *<ion>* the recombining ion, *<nn'>* denoting the parent n-shell transition class n-n'. *ls* indicates that the dielectronic data is at LS-resolution.

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.

Input Dataset

Data Root /packages/adas/adas/adf09/

Central Data | User Data   ☐ Edit Path Name

mom93#li/mom93#li_n4ls22.dat

..
mom93#li_c3ls12.dat
mom93#li_c3ls22.dat
mom93#li_c3ls23.dat
mom93#li_n4ls12.dat
mom93#li_n4ls22.dat
Data File mom93#li_n4ls23.dat
mom93#li_ne7ls12.dat
mom93#li_ne7ls22.dat
mom93#li_ne7ls23.dat

Browse Comments | Cancel | Done
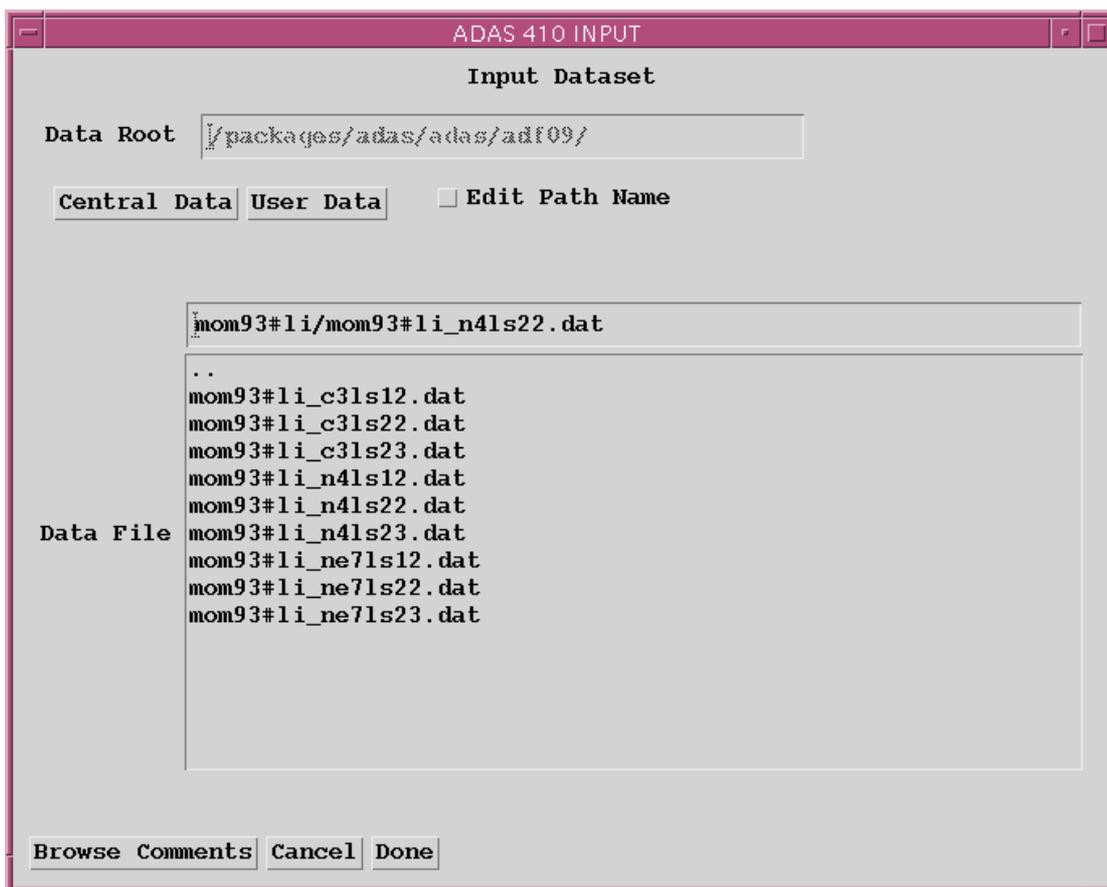
7. Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window.

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

8. An arbitrary title may be given for the case being processed. For information the full pathway to the dataset being interrogated is also shown at a). The button *Browse comments* again allows display of the information field section at the foot of the selected dataset, if it exists.

9. At b) the choice of the type of data to be extracted from the *adf09* file is selected by clicking the appropriate button. The sub-window below the buttons alters according to the choice made. The sub-window for *Representative bundle-n DR* is shown at c) and d). The schematics at f) and h) show the sub-windows for *Resolved state selective DR* and *Auger rates* respectively.

10. In the case of *Representative bundle-n DR*, select the initial parent and final parent/spin system combination first at c). Note that the dielectronic data is designed for the metastable resolved situation and so the choice of initial recombining (parent) metastable and then the recombined spin system and the parent it is built on matters. The adjacent window shows the n-shells for which data are available. These are representative n-shells up to around 1000. Data is not stored in the *adf09* file for every n-shell but only for a representative set. Codes which user the *adf09* datasets interpolate for non-representative n-shells. The selection table at d) indicates which n-shells have non-zero DR values.

11. In the case of *Resolved state selective DR*, as illustrated at f), the situation is similar. However only the initial parent is identified, since the final recombined low levels may not have a clearly distinquished parent. The initial parent is selected at f). Then the final term of the recombined ion is

selected at g). The *adf09* datasets contain fully LS resolved data for n-shells up to about 7.

12. at e), the electron temperatures at which you wish the dielectronic recombination data is chosen. Table editor is available to enter this data and default temperatures (equal to those in the *adf09* file) may be chosen by button click as usual.

13. The option of fitting a polynomial to the extracted data is offered just below the temperature selection widget.
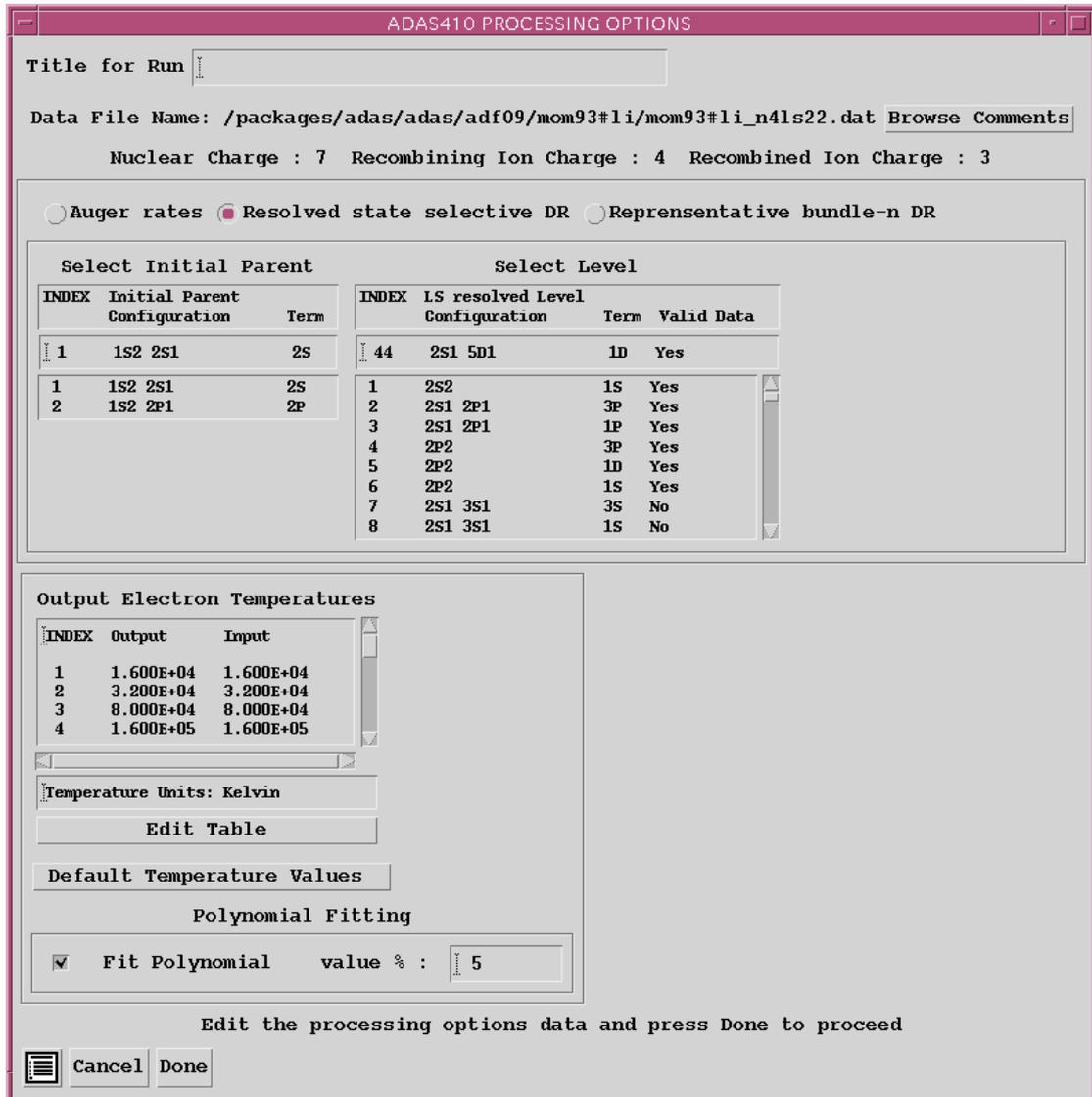
14. The Auger data is stored for representative n-shells for recombined ion parent state and final ionised ion state pairs. The data is extracted for the complete set of representative n-shells so the choice at h) is only of the initial ionising ion parent core and final ionised parent. The choices are presented at h) for selection by clicking in the usual manner.

15. 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 4 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

The **output options window** appearance is shown below

16. As in the previous window, the full pathway to the file being analysed is shown for information at a). Also the *Browse comments* button is available.

17. Graphical display is activated by the *Graphical Output* button at b). This will cause a graph to be displayed following completion of this window. When graphical display is active, an arbitrary title may be entered which appears on the top line of the displayed graph.

18. By default, graph scaling is adjusted to match the required outputs. Press the *Explicit Scaling* button at b) to allow explicit minima and maxima for the graph axes to be inserted. Activating this button makes the minimum and maximum boxes editable.

19. Hard copy is activated by the *Enable Hard Copy* button at 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.

20. A choice of output graph plotting devices is given in the Device list window to the right. Clicking on the required device selects it. It appears in the selection window above the Device list window.

21. At d) output of the tabular record of the interrogation may be enabled. This is usually called *paper.txt* and it is created in the directory from which ADAS was launched.

22. The graph is displayed in a following Graphical Output window.

23. 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 4 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.
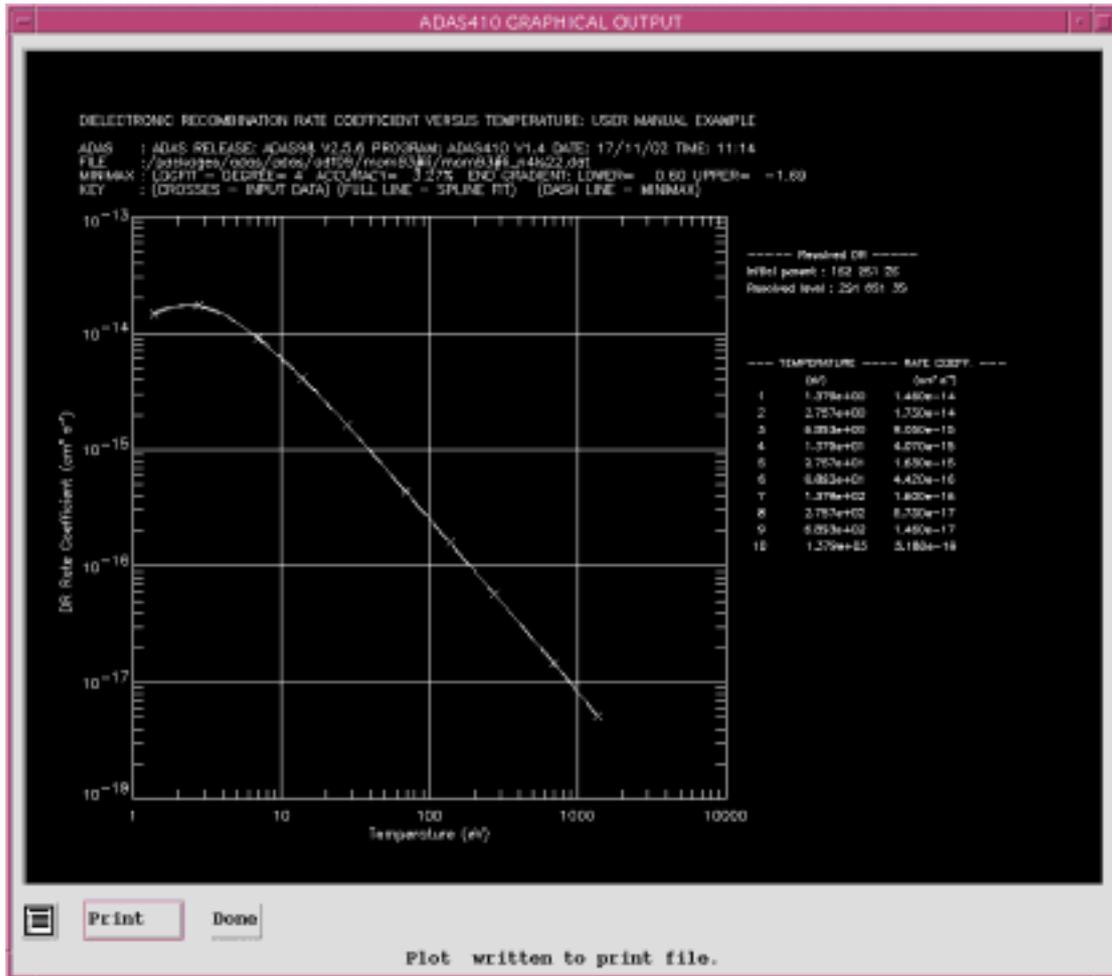
Illustration:

Figure 5.10a

DIELECTRONIC RECOMBINATION RATE COEFFICIENT VERSUS TEMPERATURE

ADAS   : ADAS RELEASE: ADAS98 V2.1 PROGRAM: ADAS410 V1.2 DATE: 25/03/99 TIME: 09:43
FILE   : /packages/adas/adas/adf09/mom93#li/mom93#li_n4ls22.dat
MINIMAX : LOGFIT − DEGREE= 3 ACCURACY= 1.79% END GRADIENT: LOWER= −0.46 UPPER= −1.40
KEY   : (CROSSES − INPUT DATA) (FULL LINE − SPLINE FIT)   (DASH LINE − MINIMAX)
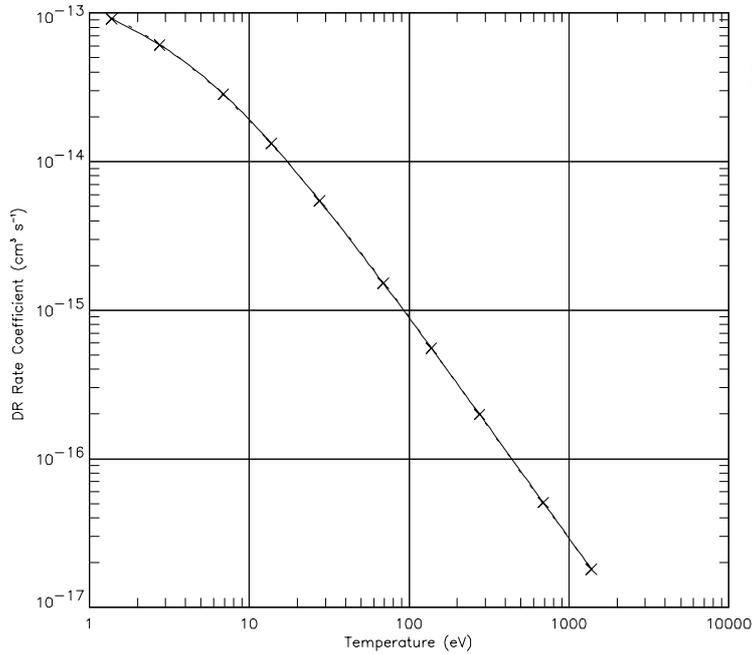
−−−−− Resolved DR −−−−−
Initial parent : 1S2 2S1 2S
Resolved level : 2S1 2P1 1P

| −−− TEMPERATURE −−−− | RATE COEFF. −−− |
| (eV) | (cm³ s⁻¹) |

	(eV)	(cm³ s⁻¹)
1	1.379e+00	9.110e−14
2	2.757e+00	6.090e−14
3	6.893e+00	2.840e−14
4	1.379e+01	1.320e−14
5	2.757e+01	5.440e−15
6	6.893e+01	1.520e−15
7	1.379e+02	5.540e−16
8	2.757e+02	1.990e−16
9	6.893e+02	5.090e−17
10	1.379e+03	1.810e−17

Table 5.10a

```
ADAS RELEASE: ADAS98 V2.1 PROGRAM: ADAS410 V1.2 DATE: 25/03/99 TIME: 09:43

**** TABULAR OUTPUT FROM DIELECTRONIC RECOMBINATION RATE-COEFFICIENT IN PROGRAM: ADAS410 - DATE:
25/03/99 ***


------------------                                        ------------------
  DIELECTRONIC RECOMBINATION  RATE-COEFFICIENTS AS A FUNCTION OF TEMPERATURE
  ----------------------------------------------------------------------------
                    DATA GENERATED USING PROGRAM: ADAS410
                    -------------------------------------
  FILE : /packages/adas/adas/adf09/mom93#li/mom93#li_n4ls22.dat


                          --------
  Element                   :  NITROGEN
  Nuclear charge        (Z0) :      7
  Recombining ion charge (Z1) :      4
  Recombined ion charge  (Z)  :      3
                          --------
  Initial parent            :  1S2 2S1        2S
  Resolved level            :  2S1 2P1        1P

-------- TEMPERATURE --------      RATE COEFFICIENT
     Kelvin      eV                cm**3/sec
    1.600D+04   1.379D+00         9.1100D-14
    3.200D+04   2.757D+00         6.0900D-14
    8.000D+04   6.893D+00         2.8400D-14
    1.600D+05   1.379D+01         1.3200D-14
    3.200D+05   2.757D+01         5.4400D-15
    8.000D+05   6.893D+01         1.5200D-15
    1.600D+06   1.379D+02         5.5400D-16
    3.200D+06   2.757D+02         1.9900D-16
    8.000D+06   6.893D+02         5.0900D-17
    1.600D+07   1.379D+03         1.8100D-17
-----------------------------------------------------------------------------
NOTE: * => RATE-COEFFICIENT EXTRAPOLATED FOR THIS TEMPERATURE VALUE
-----------------------------------------------------------------------------
-----------------------------------------------------------------------------
         A( 1) = -1.297832394D+01         A( 2) =  -3.232353745D-01
         A( 3) = -4.907472614D-01         A( 4) =   6.771810048D-02

LOGFIT - DEGREE= 3  ACCURACY=  1.79%  END GRADIENT: LOWER=  -0.46 UPPER=  -1.40
-----------------------------------------------------------------------------
```

Notes: