ADAS402: Isonuclear sequence data - graph and fit coefficient

The program interrogates iso-nuclear master files of type ADF11. It extracts collisional radiative coefficients of various classes relevant to plasma modelling stored in iso-nuclear sequence sets. The data may be interpolated using cubic splines to provide the coefficients at a selected charge state of the chosen element and at selected electron temperature/electron density pairs. A minimax polynomial approximation is also made to the data. Interpolated data and some comparative source data are displayed and a tabulation printed. The printed output includes the minimax polynomial approximation.

Background theory:

The source files to be interrogated are of both ordinary (stage to stage) and generalised (metastable resolved) collisional radiative coefficients. A file is associated with an element and a data class. There are separate files for ordinary and generalised data. The classes of data include the collisional-dielectronic recombination coefficient (ACD), the collisional-dielectronic ionisation coefficient (SCD), the collisional-radiative charge exchange recombination coefficient (CCD), the collisional-dielectronic recombination/cascade / bremsstrahlung radiated power coefficient (PRB), the collisional-radiative charge exchange recombination/cascade power coefficient (PRC), the collisional-radiative metastable cross-coupling coefficient (QCD) and the collisional-dielectronic parent cross-coupling coefficient (XCD), the collisional-radiative excitation total line power coefficient (PLT) and the collisional-radiative excitation specific line power coefficient (PLS). Altogether there are nine classes. The internal organisation of the data is different depending on whether they are stage to stage (data prefix 'U' or no prefix) or metastable resolved (data prefix 'R'). The data classes QCD and XCD do not occur in the stage to stage case. The classes are summarised below:

| Mnemonic	Class	Data prefix
ACD	Coll.-diel. recom. coefft.	R & U (or none)
SCD	Coll.-diel. ionis. coefft.	R & U (or none)
CCD	Coll.-rad. charge exch. coefft.	R & U (or none)
PRB	Coll.-diel. recom./brems. power coefft.	R & U (or none)
PRC	Coll.-rad. charge exch. recom. power coefft.	R & U (or none)
QCD	Coll.-rad. metastable cross coupling coefft.	R
XCD	Coll.-diel. parent meta. cross-coupling coefft.	R
PLT	Coll.-rad. excit. line power coefft.	R & U (or none)
PLS	Coll.-rad. specific line excit. power coefft.	R & U (or none)

The span and density of N_e and T_e values in the data set are designed to minimise the need for elaborate interpolation and extrapolation. In application, linear interpolation is in general sufficiently accurate and data extraction is very rapid. However, for the interrogation program, the data are interpolated by cubic splines in the order N_e, T_e. The interpolations are carried out in the log/log plane with zero curvature end conditions on the splines.

The program accepts a set of electron temperature/electron density pairs at which the collisional radiative coefficient data are produced. The output is therefore suited to giving the run of a coefficient through a density/temperature plasma model 'atmosphere'. A minimax polynomial approximation to the output is also provided. In the display graphs, it is possible to show coefficient curves for adjacent ions of the iso-nuclear sequence to the one sought. This data is taken directly from the database, without interpolation, at the available temperatures and at one density only. Such data should be viewed as an assistance in verifying that the interpolation has proceeded satisfactorily.

Program steps:

These are summarised in figure 5.2.

Figure 5.2
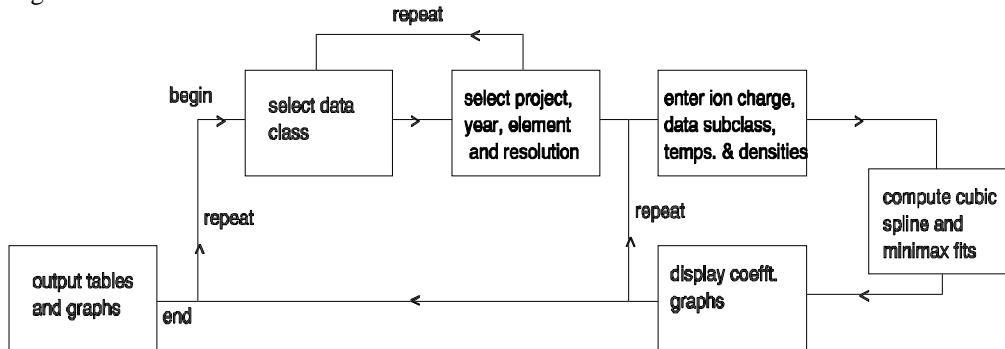
Interactive parameter comments:

Move to the directory in which you wish any ADAS created files to appear. These include the output text file produced after executing any ADAS program (*paper.txt* is the default) and the graphic file if saved (e.g. *graph.ps* if a postscript file). Initiate ADAS and move to the series 4 menu. Select ADAS402.

The **file selection window** is illustrated below. Conventional file selection and selection via a directed search are possible.
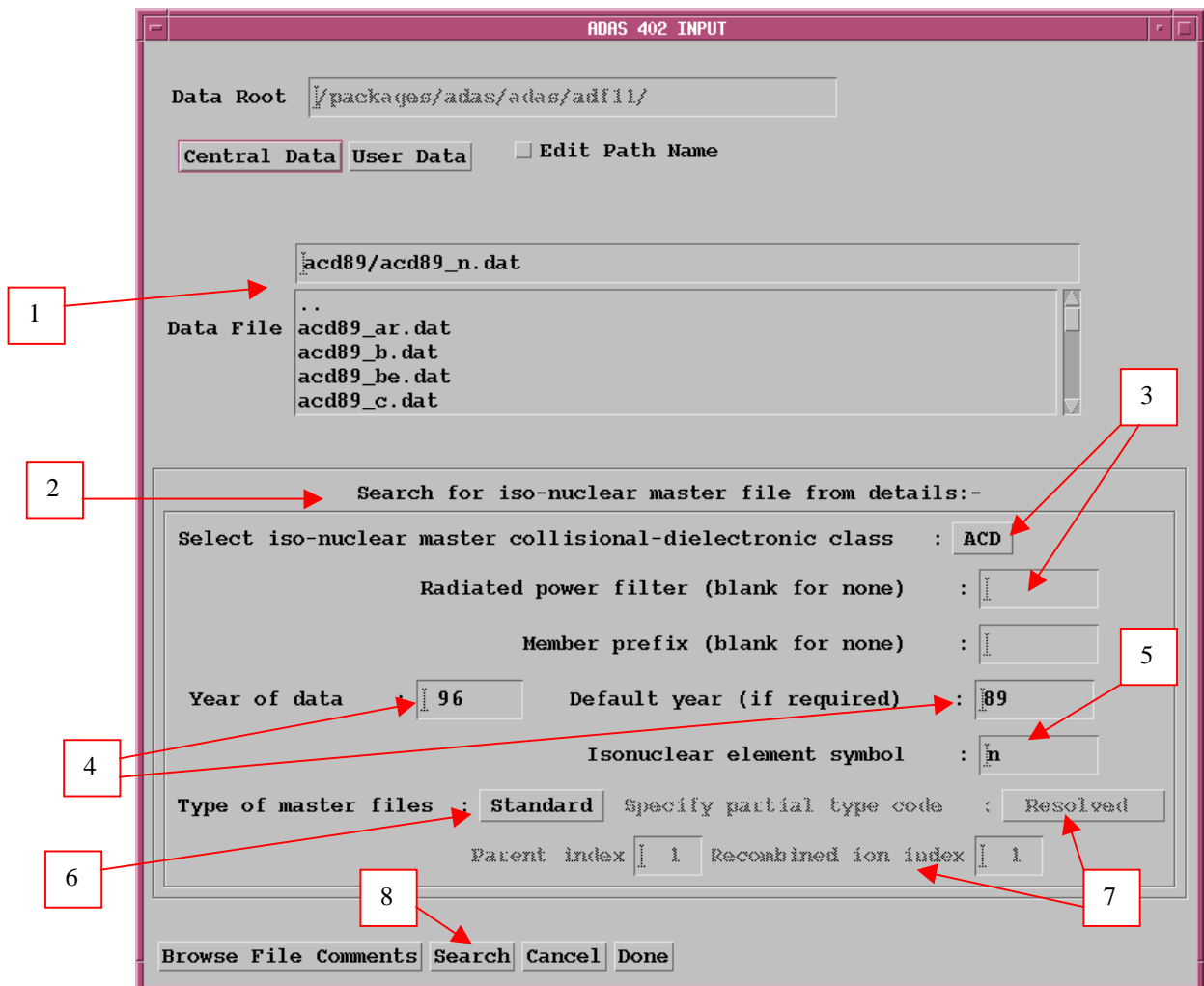
1. Buttons are present to set the data root to that of the *Central data* or to your personal *User data* (provided it is in ADAS organisation. Alternatively the 'data root' may be edit explicitly. Available data sets are shown in the file display window. Selection is made by clicking on the appropriate name, whereupon it appears in the selection window above.

2. There are very many data sets of type *adf11* grouped by year, element and data class. A search strategy is available based on initial identification of an group of files of particular year and type and then conventional selection from the group list.

3. For dataset search, select the iso-nuclear master class first. A drop-down menu is offered. The radiated power data classes (PLT, PRB and PRC) can include the attenuation due to an energy filter. Enter the filter if required. At this stage only a very limited amount of filtered power data has been placed on the workstation database. The naming convention is defined in the *adf11* specification. To allow further distinction of data within the same year, a prefix can be used within the dataset name structure (eg. *acd93r_<prefix>_o.dat*). Enter this if required at *Member prefix*.

4. Enter the two-digit year number of the data required at *Year of data* . A *Default year* may be entered which will be used if there is no data of the required class in the *Year of data*.

5. Enter the *Iso-nuclear sequence symbol*.

6. There are two primary organisations of adf11 data, Standard (ionisation stage to ionisation stage) and Partial (metastable to metastable). Select the type required in the drop-down menu at *Type of master file*.

7. If Partial is chosen, further selections may be made. Within the Partial type of organisation, true metastable to metastable subdivided data is called Resolved. Stage to stage data can be written into the Partial type of structure and is then called Unresolved. This un-necessary duplication is because of a historical precedent in IBM-ADAS at JET. Select as required in the drop-down menu at *Specify partial type code.* Finally within the Resolved type enter the particular metastable to metastable sought at *Parent index* and *Recombined ion index*. Note that the items selected here are only used when the dataset is opened at the Processing Options stage.

8. Initiate the search for the required dataset sub-list by clicking *Search* .

The **search result window** has the appearance shown above
1. If there is a choice of files, click on the one you wish.
2. Return to the input window by clicking *Select*.
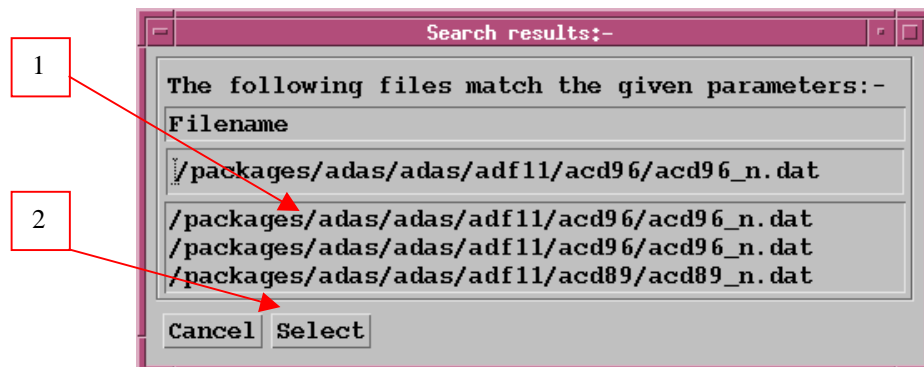
The **processing options window** has the appearance shown below

1. Data file and iso-nuclear sequence information is given.
2. A particular charge state of the iso-nuclear sequence should be selected. This is by entering any one of the three fields, namely, element nuclear charge (nuclear charge number or symbol), recombining ion charge or recombined ion charge
3. The extracted data is interpolated by a cubic spline to the selected ion and user temperature/density pairs for graphical display and tabular output. Additionally a polynomial approximation may obtained by making the appropriate selections.
4. Select temperature and density pairs for data output (Output). The source data is held in two-dimensional arrays, that is as a function of electron temperature and electron density. The source (Input) values are also shown. The table may be edited by clicking on the *Edit Table* button.. The ADAS Table Editor window is then presented with usual set of editing operations available.
5. The displayed graph of the interpolated coefficient as a function of electron temperature also shows some additional curves from the dataset for comparison. These additional curves are drawn directly from the dataset and are not interpolated. Thus they must be at fixed electron density. Specify the *Approximate density to be extracted.* The nearest fixed density in the dataset will be used for the comparative curves.
6. Clicking the *Done* button causes the next output options window to be displayed. Remember that *Cancel* takes you back to the previous window. The *Escape to Menu* icon is also available for a quick exit at the bottom left hand corner.
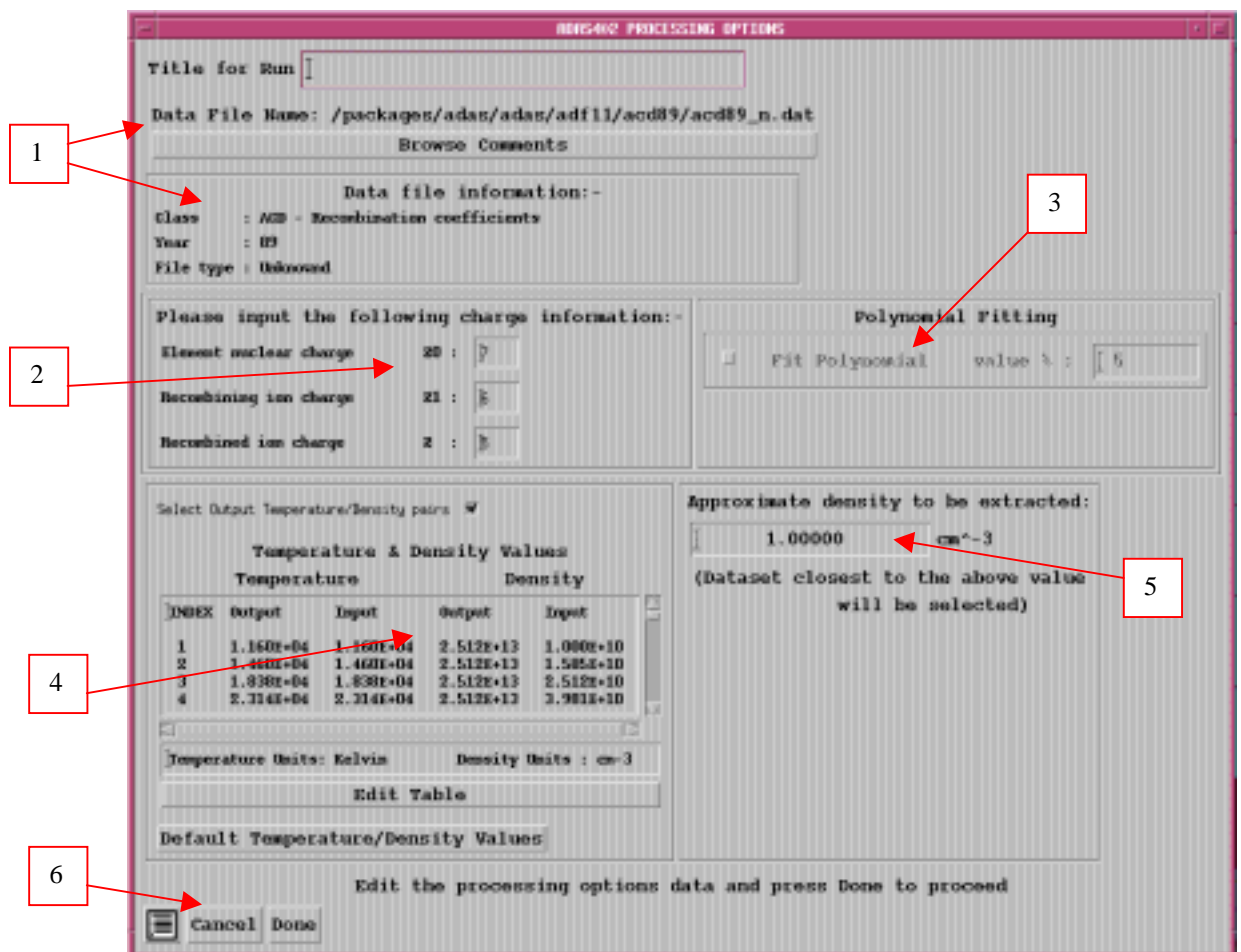
The **Output options window** is shown below. Broadly it follows the pattern of other ADAS interrogation codes.

1. Graphical output is enabled by clicking on the button. Default scaling of graphs may be over-ridden by appropriate selections.
2. Hard copy may be enabled and the type of output device selected.
3. As usual a line printer text output file summarising the interrogation may be produced.
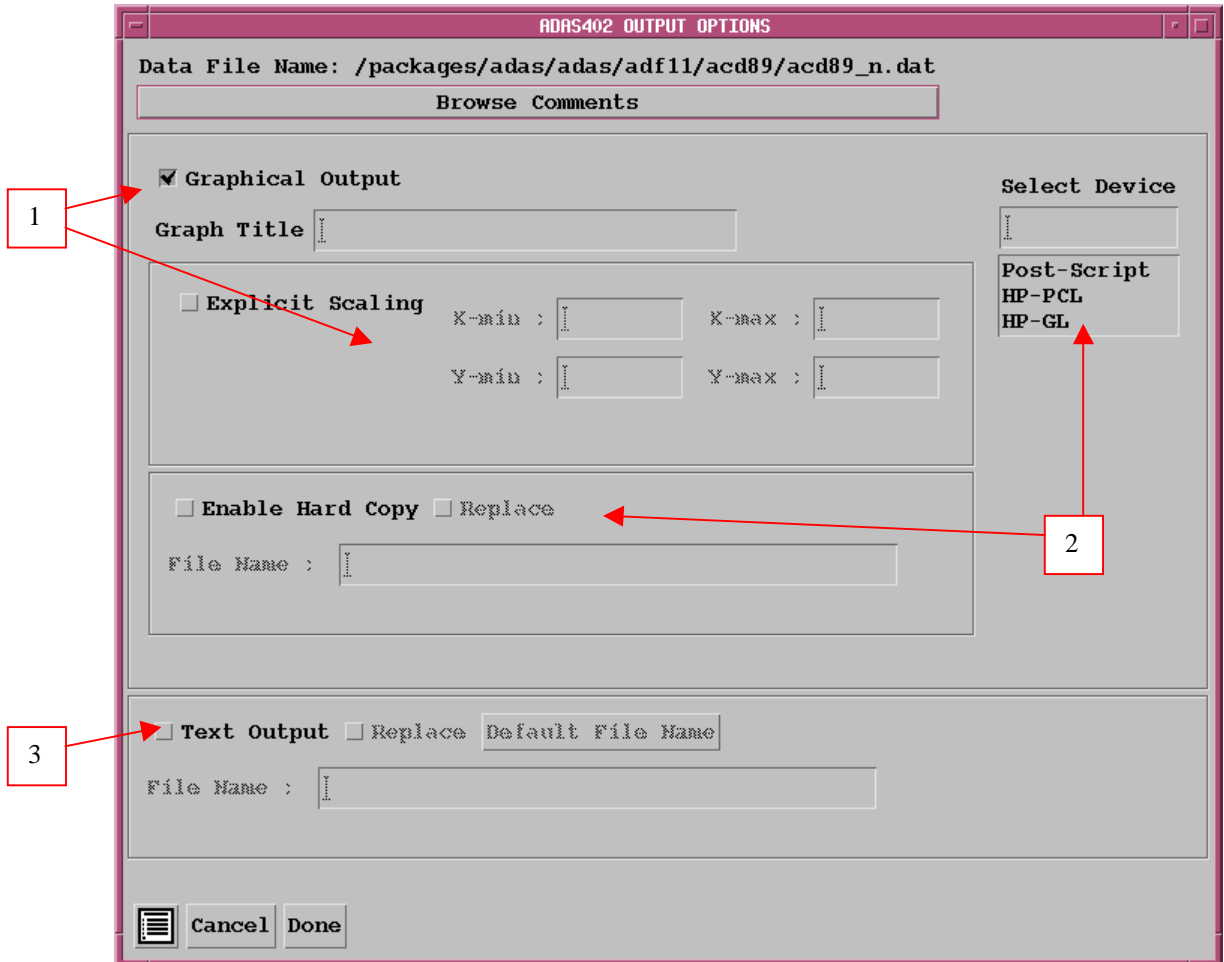
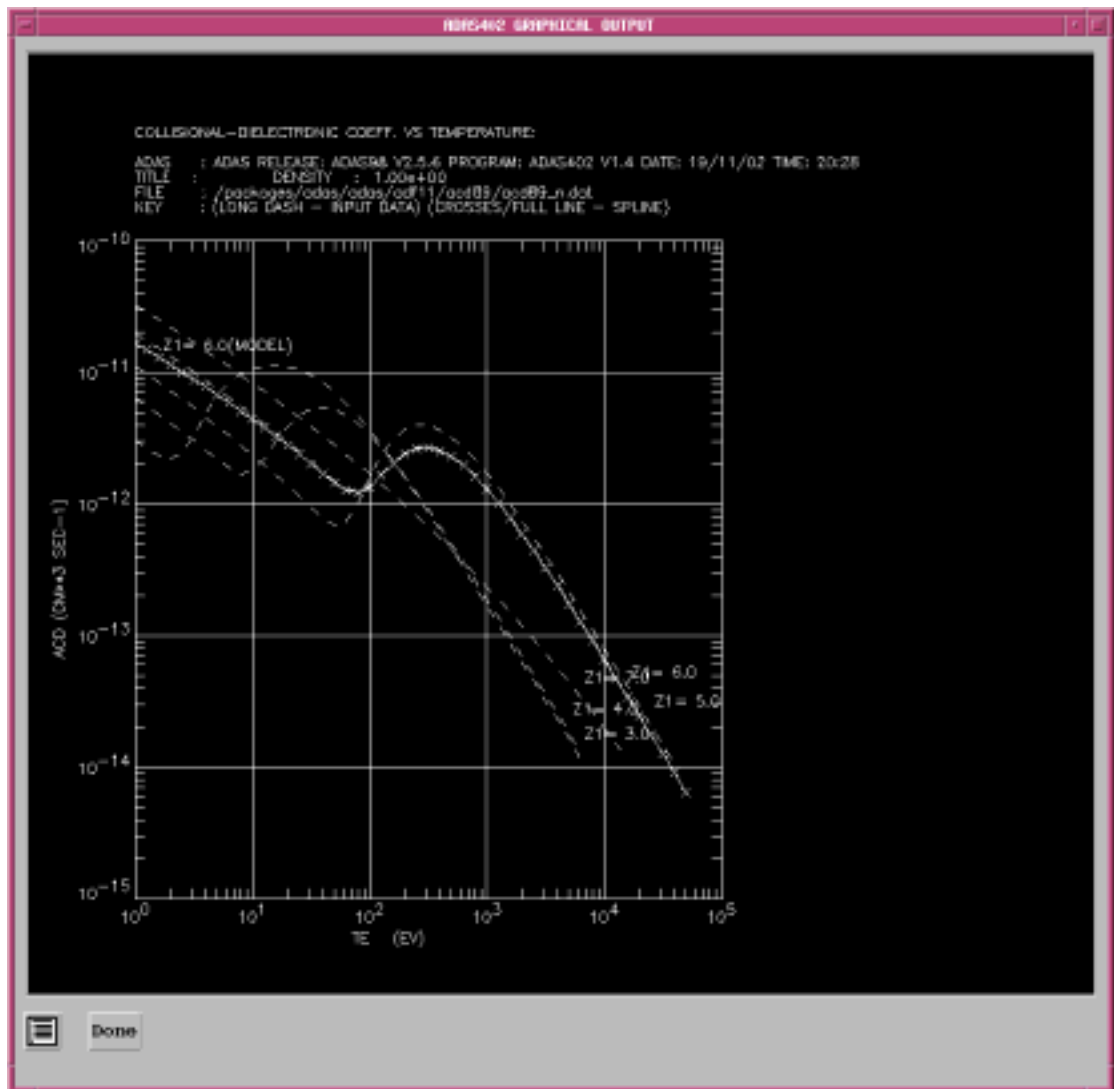The **graphical output** is as shown below.

Illustration:

The output from the program is illustrated for the collisional-dielectronic recombination coefficient of the member O^{+6} of the oxygen iso-nuclear sequence, recombining to form the lithium-like ion O^{+5}. A standard unresolved master file data set is used. The graph shows also a number of adjacent ionisation stages.

Figure 5.2a

OXYGEN ACD STUDY   28/08/92
FILE = /JETSHP.ACD89#O.DATA   DENSITY = 2.51D+13 CM-3
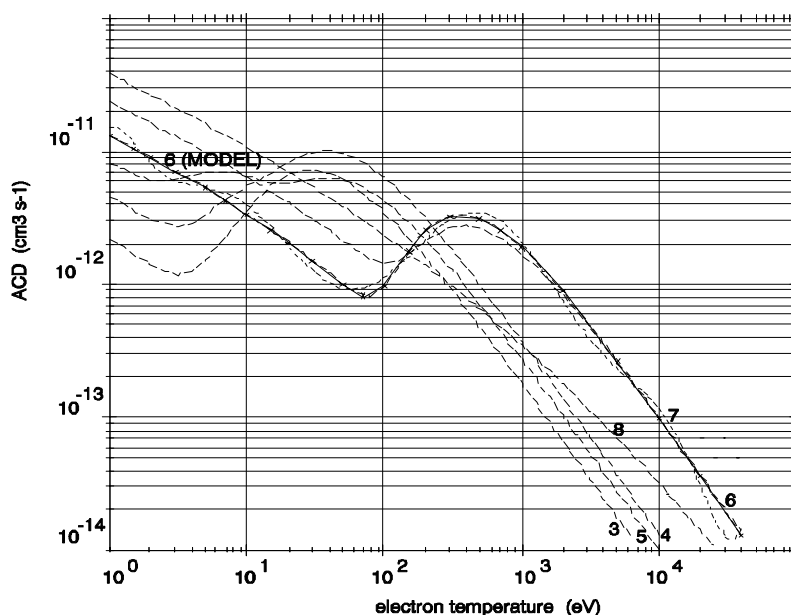LOGFIT - DEGREE = 9 ACCURACY = 17.63% END GRADIENT LOWER = 0.54 UPPER = 3.02

Table 5.2a

```
                                OXYGEN ACD STUDY      28/08/92)
 DATA GENERATED USING PROGRAM ADAS402
 ------------------------------------
 NUCLEAR CHARGE =  8.00     RECOMBINING ION CHARGE =  6.00      RECOMBINED ION CHARGE
=  5.00
 FILE = /JETSHP.ACD89#O.DATA              DENSITY   =  2.51D+13 CM-3

       TEMP(K)        TEMP(EV)        TEMP(K)/Z1**2     DENS(CM-3)       RATE COEFF(CM**3/S)
     ---------      ---------       -------------     ----------       -------------------
     1.160D+04      1.000D+00         3.222D+02        3.000D+13               1.304D-11
     1.740D+04      1.500D+00         4.833D+02        3.000D+13               1.037D-11
     2.320D+04      2.000D+00         6.444D+02        3.000D+13               8.965D-12
     3.480D+04      3.000D+00         9.667D+02        3.000D+13               7.061D-12
     5.800D+04      5.000D+00         1.611D+03        3.000D+13               5.250D-12
     8.120D+04      7.000D+00         2.256D+03        3.000D+13               4.213D-12
     1.160D+05      1.000D+01         3.222D+03        3.000D+13               3.343D-12
     1.740D+05      1.500D+01         4.833D+03        3.000D+13               2.511D-12
     2.320D+05      2.000D+01         6.444D+03        3.000D+13               2.058D-12
     3.480D+05      3.000D+01         9.667D+03        3.000D+13               1.501D-12
     5.800D+05      5.000D+01         1.611D+04        3.000D+13               1.002D-12
     8.120D+05      7.000D+01         2.256D+04        3.000D+13               8.179D-13
     1.160D+06      1.000D+02         3.222D+04        3.000D+13               9.607D-13
     1.740D+06      1.500D+02         4.833D+04        3.000D+13               1.769D-12
     2.320D+06      2.000D+02         6.444D+04        3.000D+13               2.544D-12
     3.480D+06      3.000D+02         9.667D+04        3.000D+13               3.266D-12
     5.800D+06      5.000D+02         1.611D+05        3.000D+13               3.095D-12
     8.120D+06      7.000D+02         2.256D+05        3.000D+13               2.548D-12
     1.160D+07      1.000D+03         3.222D+05        3.000D+13               1.887D-12
     2.320D+07      2.000D+03         6.444D+05        3.000D+13               8.800D-13
     5.800D+07      5.000D+03         1.611D+06        3.000D+13               2.641D-13
     1.160D+08      1.000D+04         3.222D+06        3.000D+13               9.916D-14
     2.320D+08      2.000D+04         6.444D+06        3.000D+13               3.623D-14
     4.640D+08      4.000D+04         1.289D+07        3.000D+13               1.306D-14


 TAYLOR COEFFICIENTS OF MINIMAX POLYNOMINAL  ( LOG10(RATE COEF) VS LOG10(TEMP(EV))
 --------------------------------------------------------------------------------

     1) =  -1.081408270D+01      2) =   5.418948485D-01      3) =  -1.170001862D+01
     4) =   3.362251493D+01      5) =  -4.419515956D+01      6) =   3.099482897D+01
     7) =  -1.232626522D+01      8) =   2.789343502D+00      9) =  -3.349773410D-01
    10) =   1.658318363D-02
 LOGFIT - DEGREE= 9  ACCURACY= 17.63%  END GRADIENT: LOWER=   0.54 UPPER=   3.02
```

Notes: