ADAS401: Isoelectronic sequence data - graph and fit coefficient

The program interrogates iso-electronic master files of type ADF10. It extracts collisional radiative coefficients of various classes relevant to plasma modelling stored in isoelectronic sequence sets. The data may be interpolated using cubic splines to provide the coefficients at a selected charge state and arbitrary 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 contain both ordinary (stage to stage) and generalised (metastable resolved) collisional radiative coefficient. The files of ordinary type are called *standard files* (S) and the files of generalised type are called *partial files* (P) here. The classes of data in the partial files 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). For the standard files, the QCD and XCD data classes do not occur. Altogether there are nine classes. The internal organisation of the data in the files is according to two categories namely *recombination/ionisation* (*RI*) and *line/power* (*LP*). The classes are summarised below:

Mnemonic	Class	Forms	Categories
ACD	Coll.-diel. recom. coefft.	P & S	RI
SCD	Coll.-diel. ionis. coefft.	P & S	RI
CCD	Coll.-diel. charge exch. coefft.	P & S	RI
PRB	Coll.-diel. recom./brems. power coefft.	P & S	RI
PRC	Coll.-rad. charge exch. recom. power coefft.	P & S	RI
QCD	Coll.-rad. metastable cross coupling coefft.	P	RI
XCD	Coll.-diel. parent meta. cross-coupling coefft.	P	RI
PLT	Coll.-rad. excit. line power coefft.	P & S	LP
PLS	Coll.-rad. specific line excit. power coefft.	P & S	LP

The interrogation program accesses the various data classes. It then interpolates the data using cubic splines to provide results for a selected class of collisional-dielectronic coefficient for a selected charge state, for a selected metastable sub-class in the partial case, and for selected electron temperature/electron density pairs within the range of the datasets.

The primary calculations for collisional-radiative data are carried out for a series of ions of an iso-electronic sequence at an array of electron temperatures. Advantage is taken of the regularity of coefficients along the sequence as well as in temperature and density to provide reasonably compact data sets of type ADF10 which may be interpolated in charge state, temperature and density. For accuracy in these interpolations it is important to take note of the approximate z-scaling properties of collisional-radiative coefficients. Firstly comparison of data for different charge states should be done at equal *z-scaled* (reduced) temperatures $\theta = T_e / z_1^2$ and densities $\rho = N_e / z_1^7$ where z_1-1 is the charge of the (recombined or ionising) ion. Then a constant s may be identified such that $z_1^s R_{CR}(\theta, \rho, z_1)$ is a slowly varying function of z_1 (R_{CR} denotes any collisonal-radiative coefficient). A standard set of reduced electron temperatures and densities is used for the calculation of primary data for different members of an iso-electronic sequence. The choice of a set of z_1's for satisfactory interpolability is important. It is necessary for the set to be dense at low z_1, particularly z_1=1,

2, 3 should be present. A typical set might then include z_1=5, 7, 9, 14, 20, 30. It is also helpful to supplement the data set with important ions such the carbon, oxygen, silicon, calcium, iron and nickel members as appropriate. For interpolation of data which has an exponential behaviour at low temperatures due to a finite threshold for the process, such as collisional-radiative excitation and ionisation, it is necessary to cancel the dominant temperature dependence by multiplying the coefficient values by a factor of the form $\exp((I / z_1^2) / k\theta)$, where I is an appropriate energy, prior to interpolation. The iso-electronic master files used in this work contain a set of such excitation or ionisation energies for every charge state of the iso-electronic sequence (extrapolated for z_1>50) when necessary. This is so for SCD, PLT, PLS and some QCD data sets.

Subject to these provisions, data is interpolated by cubic splines in the order, z_1, ρ and θ. The span of ρ and θ values in the data set is designed to minimise the need for extrapolation. However the end conditions at the first and last spline knots are set to give continuity onto the asymptotic behaviours where known. For each class of data the spline end conditions (1st. or 2nd. derivatives at the first and last knots) are individually set for asymptotic matching. The choices are as as follow:

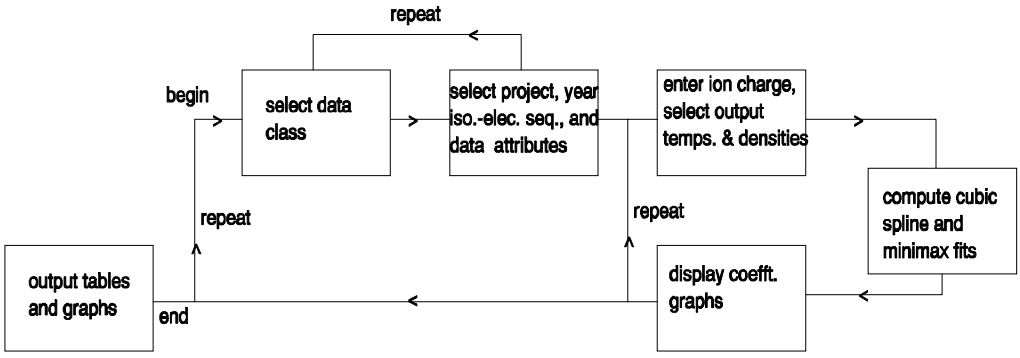
Iopt	Nopt	$\left.\frac{dy}{dx}\right\|_1$	$\left.\frac{d^2y}{dx^2}\right\|_1$	$\left.\frac{dy}{dx}\right\|_n$	$\left.\frac{d^2y}{dx^2}\right\|_n$	Extrapol.
< 0	0	.	0.0	.	0.0	no
0	0	.	0.0	.	0.0	yes
1	1	.	0.0	-1.5	.	yes
2	2	0.0	.	1.0	.	yes
3	3	-0.5	.	-1.5	.	yes
4	4	0.0	.	.	0.0	yes

Iopt and Nopt are the controlling switches for extrapolation and end conditions permission respectively in the spline routines.

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 nearest neighbour members of the isoelectronic sequence to the one sought. This data is taken directly from the database, without interpolation, at the available reduced temperatures and at one reduced density only. Such data should be viewed as an assistance in verifying that the interpolation has proceeded satisfactorily. Also, in assembling iso-electronic master files, the display may give guidance on increasing the density of z_1 values.

Program steps:

Figure 5.1

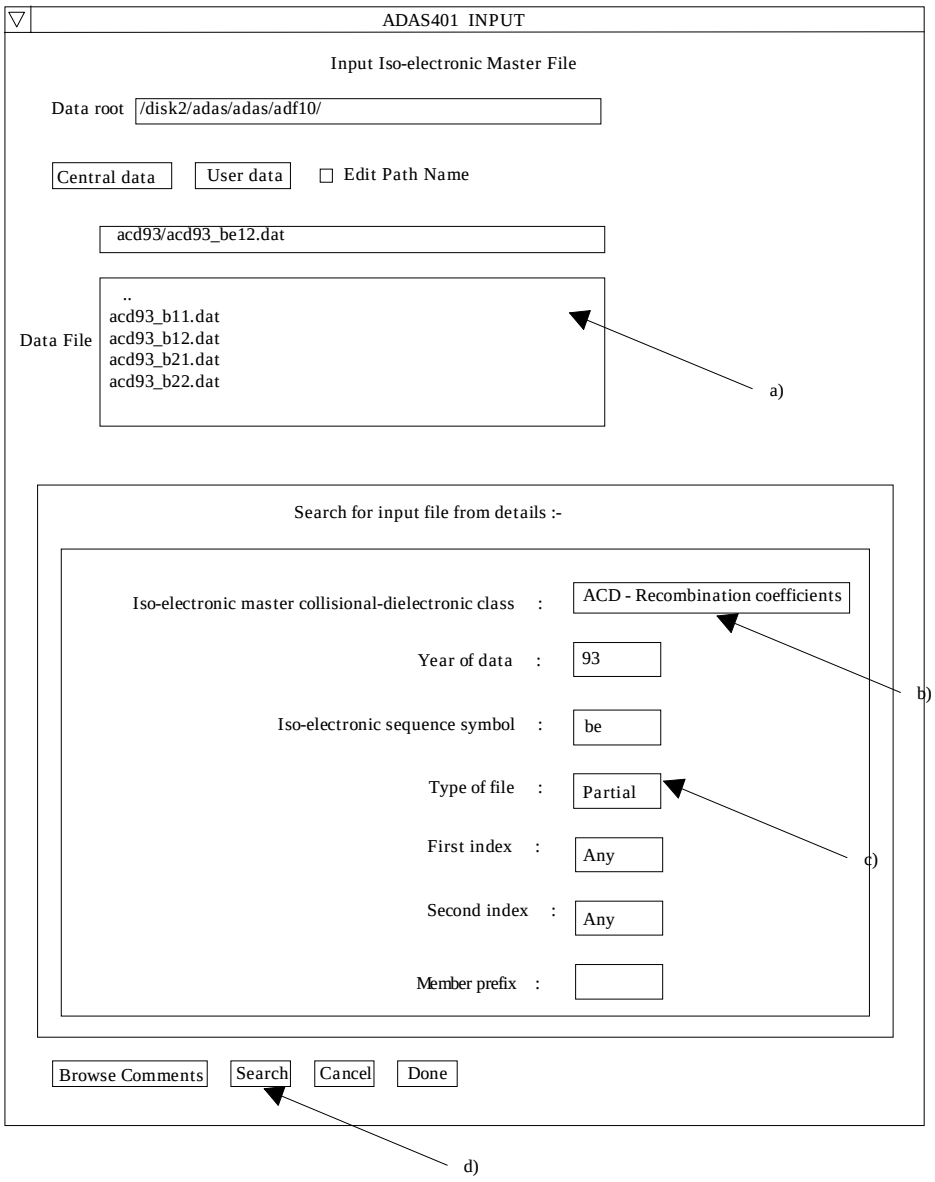


Interactive parameter comments:

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). Inititate ADAS and move to the series 4 menu. Select ADAS401.

The **file selection window** appears first and is illustrated below. Its operation is somewhat more elaborate than the standard one (cf. bulletin *jan18-95*).

1. *adf10* is the appropriate format for use by the program ADAS401 (ADAS User Manual, *appxb-10*). Your personal data of this type should be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas.*



2. Available sub-directories and data files are shown in the file display window (a). Selection is made by clicking on the appropriate name whereupon it appears in the selection window above. 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.

3. ADAS401 relies on the structure of the file name file to identify the organisation of the data within it. The key fields lie between the underscore, '_' and '*.dat*' parts of the file name (a). The characters (eg. be or b) specify the isoelectronic sequence, that is the (lower case) chemical symbol of the first member of the sequence. If no digits follow the chemical symbol, the file is of standard type. Otherwise the data set is of partial type and there are two digits indexing initial and final metastable states. The

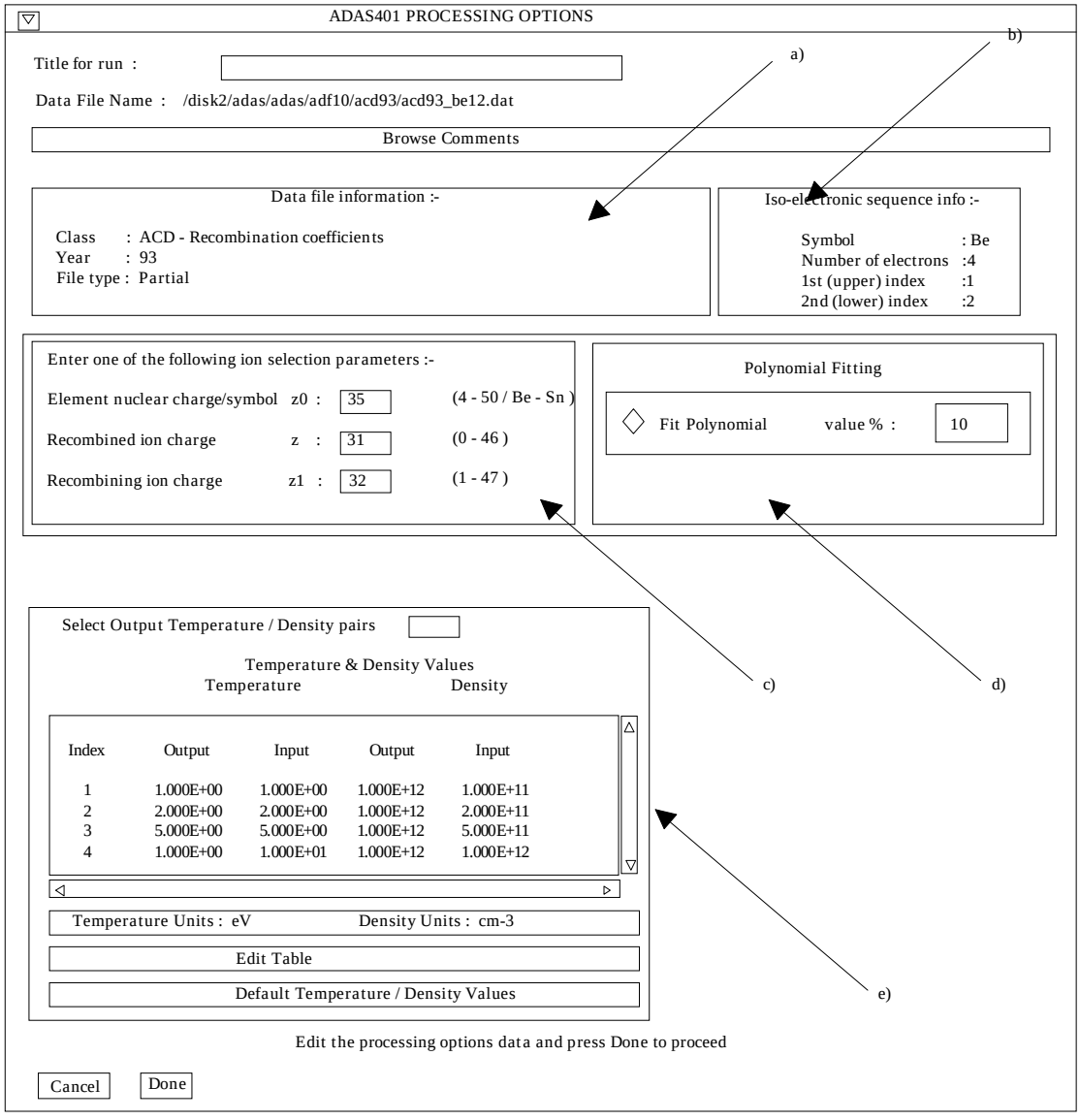
exact definitions are given in the User Manual. **There is a known error. Data of type PLT in the partial case has the digits replaced by '##'. Such data cannot be interrogated at this time by ADAS401.**

4. To ease file selection, an alternative strategy is available. Central ADAS data makes use of the data class in lower case (eg. '*acd*') and a two digit year number (eg. '*93*') to assemble a standardised file name such as shown at (a). Files can be located by specifying these name parts in the 'Search for input file details' window. Click on the appropriate boxes to present either a drop down choice or to make the window editable (cf. (b) and (c)). Click the Search button to present a list of files satisfying the entered fields in the Data File window at (a). Thus '*Any*' may be entered for the First index or Second index to show all partial files for the selected sequence and year.

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.

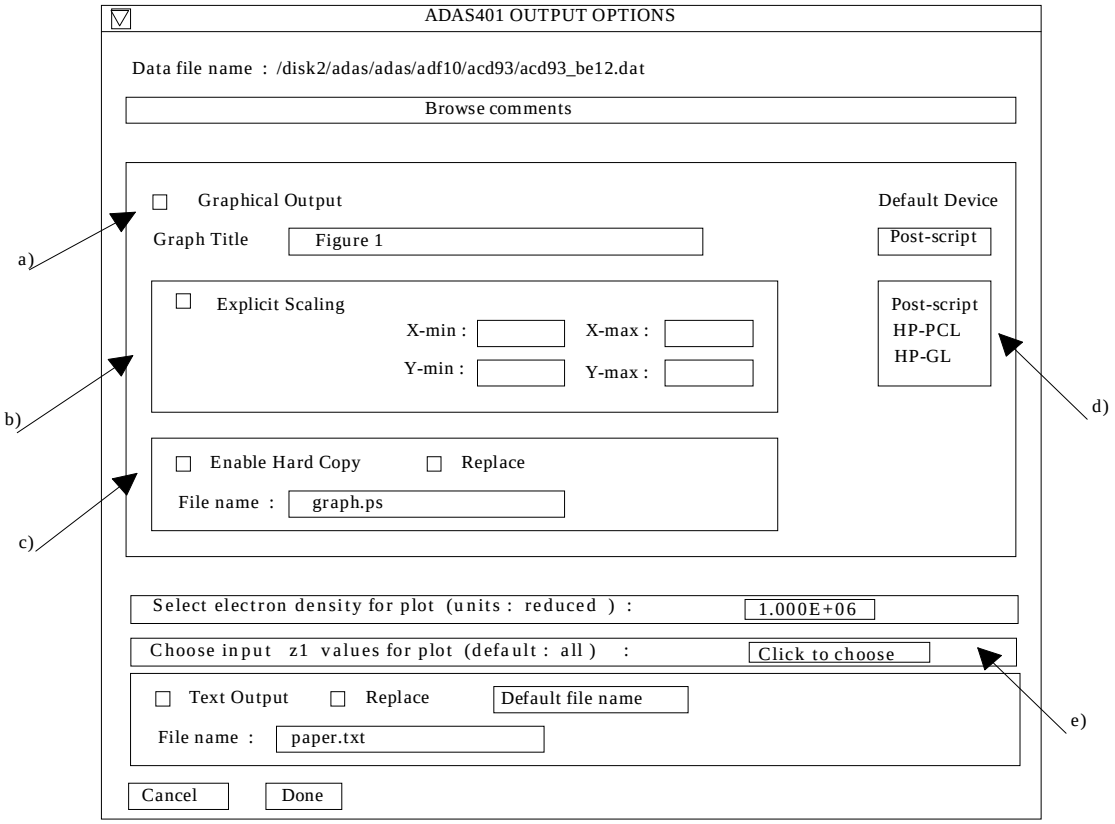
The **processing options window** has the appearance shown below



7. Data file information is given at (a) and iso-electronic sequence information at (b).

8. A particular member of the iso-electronic sequence is selected at (c). This is by entering any one of the three fields, namely, element nuclear charge (nuclear charge number or symbol), recombined ion charge or recombining ion charge. **Remember to press *Return* after entering a value in an editable window.**
9. 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 at (d).
10. Data file information is given at (a) and iso-electronic sequence information at (b).
11. A particular member of the iso-electronic sequence is selected at (c). This is by entering any one of the three fields, namely, element nuclear charge (nuclear charge number or symbol), recombined ion charge or recombining ion charge. **Remember to press *Return* after entering a value in an editable window.**
12. 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 at (d).
13. The selection of temperature and density pairs for data output are made at (e). The source data is held in two-dimensional arrays, that is as a function of z-scaled electron temperature and z-scaled electron density. The source values are also shown at (e). The table may be edited by clicking on the *Edit Table* button.. The ADAS Table Editor window is then presented with the same set of editing operations available as are described in bulletin *nov18-94*.
14. Clicking the *Done* button causes the output options window to be displayed. Remember that *Cancel* takes you back to the previous window.

The **Output options window** is shown below. Broadly it follows the pattern of other ADAS interrogation codes.



15. Graphical output is enabled by clicking on the button at (a). Default scaling of graphs may be over-ridden by appropriate selections at (b). Hard copy may be enabled at (c) with the type of output device selected at (d).

16. In addition to the plot of data according to the user values of ion, temperature, density etc. entered on the Processing Option window, additional plots of adjacent data may be made on the same graph. This is to give some guidance on the accuracy of interpolations and whether the *adf10* grids are sufficient dense for particular user tasks. Adjacent members of the iso-electronic sequence to the ion sought by the user, present in the source data set, may be shown. Click at (e) to drop down a selection list of available ions. The supplementary plots can only be provided at an electron density for which data are present in the source file. Select this density in the window above (e).

17. As usual a line printer text output file summarising the interrogation may be produced.

Illustration:

The output from the program is illustrated for the generalised collisional-dielectronic recombination coefficient of the member O^{+5} of the lithium-like iso-electronic sequence, recombining to form the beryllium-like ion O^{+4}. For this sequence, metastable resolved data is present and the results are for the 2s ^{2}S initial (parent) state and 2s^2 ^{1}S final metastable state.

Figure 5.1a

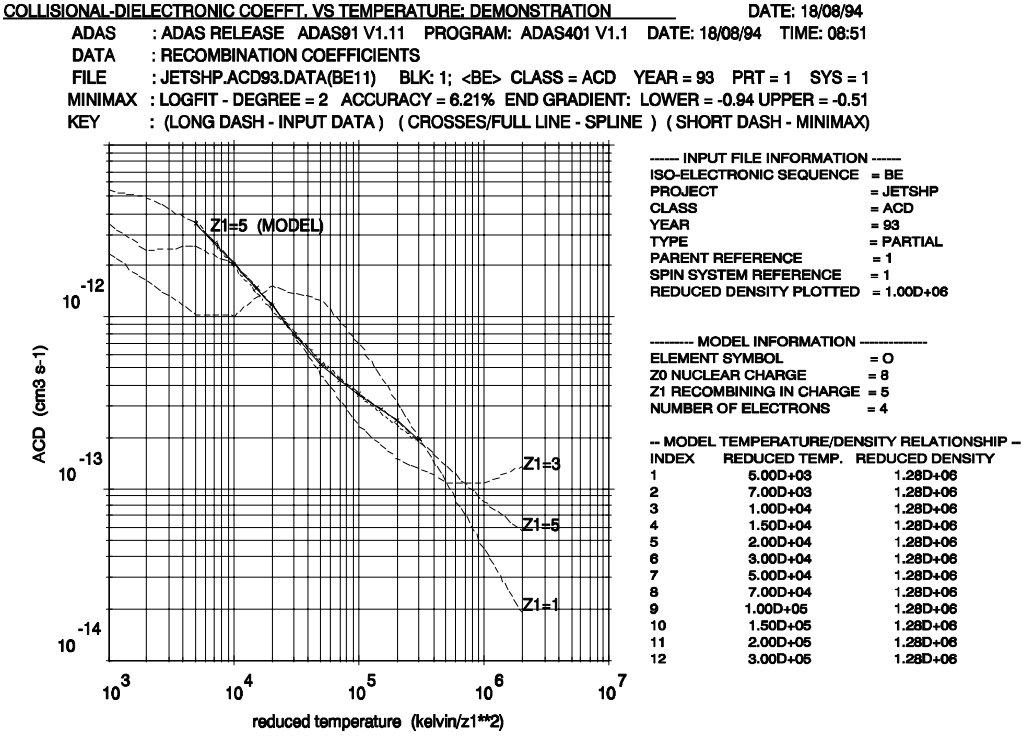


Table 5.1a

```
 ADAS RELEASE: ADAS91 V1.11  PROGRAM: ADAS401 V1.1   DATE: 18/08/94  TIME: 08:57
 ****** TABULAR OUTPUT FROM  ISO-ELECTRONIC SEQUENCE INTERROGATION PROGRAM: ADAS401 - DATE: 18/08/94
********

 -------------------- DEMONSTRATION  18/08/94                  --------------------
  RATE COEFFICIENT AS A FUNCTION OF ELECTRON TEMPERATURE AND DENSITY
  ------------------------------------------------------------------------
                  DATA GENERATED USING PROGRAM: ADAS401
                  -------------------------------------
 FILE: JETSHP.ACD93.DATA(BE11)
 DATA: RECOMBINATION COEFFICIENTS
 INPUT FILE INFORMATION:
 -----------------------
 ISO-ELECTRONIC SEQUENCE     =  BE
 PROJECT                     =  JETSHP
 CLASS                       =  ACD
 YEAR                        =  93
 TYPE                        =  PARTIAL
 PARENT REFERENCE            =   1
 SPIN SYSTEM REFERENCE       =   1
 MODEL INFORMATION:
 ------------------
```

```
 ELEMENT NAME                =  OXYGEN
 ELEMENT SYMBOL              =  O
 NUCLEAR CHARGE         (Z0) =    8
 RECOMBINING ION CHARGE (Z1) =    5
 RECOMBINED  ION CHARGE (Z)  =    4
 NUMBER OF ELECTRONS         =    4

  ------ ELECTRON TEMPERATURE ------    -- ELECTRON DENSITY --    RATE-COEFFICIENT
     kelvin        eV       K/Z1**2       cm-3     cm-3/Z1**7       cm**3/sec
   1.250D+05   1.077D+01   5.000D+03    1.000D+11   1.280D+06      3.426D-12
   1.750D+05   1.508D+01   7.000D+03    1.000D+11   1.280D+06      2.695D-12
   2.500D+05   2.154D+01   1.000D+04    1.000D+11   1.280D+06      2.033D-12
   3.750D+05   3.231D+01   1.500D+04    1.000D+11   1.280D+06      1.472D-12
   5.000D+05   4.308D+01   2.000D+04    1.000D+11   1.280D+06      1.157D-12
   7.500D+05   6.463D+01   3.000D+04    1.000D+11   1.280D+06      8.018D-13
   1.250D+06   1.077D+02   5.000D+04    1.000D+11   1.280D+06      5.235D-13
   1.750D+06   1.508D+02   7.000D+04    1.000D+11   1.280D+06      4.242D-13
   2.500D+06   2.154D+02   1.000D+05    1.000D+11   1.280D+06      3.537D-13
   3.750D+06   3.231D+02   1.500D+05    1.000D+11   1.280D+06      2.895D-13
   5.000D+06   4.308D+02   2.000D+05    1.000D+11   1.280D+06      2.484D-13
   7.500D+06   6.463D+02   3.000D+05    1.000D+11   1.280D+06      1.942D-13
 -------------------------------------------------------------------------------
 NOTE: * => RATE-COEFFICIENT EXTRAPOLATED FOR TEMPERATURE/DENSITY VALUE
 -------------------------------------------------------------------------------

0MINIMAX POLYNOMIAL FIT - TAYLOR COEFFICIENTS:
 -------------------------------------------------------------------------------
 - LOG10(RATE COEFFICIENT<cm**3/sec>) vs. LOG10(ELECTRON TEMPERATURE<K/Z1**2>) -
 -------------------------------------------------------------------------------
           A( 1) =  -6.347068876D+00            A( 2) =  -1.818070930D+00
           A( 3) =   1.193468921D-01
 LOGFIT - DEGREE= 2  ACCURACY=  6.21%  END GRADIENT: LOWER=  -0.94 UPPER=  -0.51
 -------------------------------------------------------------------------------
```

Notes