

ADAS309: Charge exchange spectroscopy - process effective coefficients: l-resolved/scan

The program computes sets of effective emission coefficients for transitions in hydrogen-like impurities following charge exchange recombination from neutral beam donors. The coefficients are for principal quantum shell transitions obtained by summation of partial coefficients from an nl-resolution collisional-radiative model. They are prepared over one-dimensional scans of plasma parameters around a reference set and assembled directly to the data format specification ADF12.

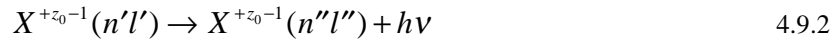
Background theory:

The code is variant of ADAS308 where a full theoretical description is given. It is designed to provide tabulations of effective emission coefficients only and excludes analysis of observed line-of-sight spectral emissivities and display.

Charge exchange spectroscopy is driven by reactions of the form



in which an electron is captured from a donor atom in its ground (or an excited) state. The principal application is usually to capture by the bare nuclei of impurity atoms in the plasma from the ground state of deuterium, helium or lithium atoms in fast neutral beams. Subsequently the hydrogen-like impurity ion radiates as



Composite spectral line features of the form $n' \rightarrow n''$ are observed made up from unresolved $n'l' \rightarrow n''l''$ multiplets. The code computes $q_{n \rightarrow n'}^{(eff)}$, the *effective emission coefficient* for the whole $n \rightarrow n'$ principal quantum shell transition, where

$$\begin{aligned} q_{n \rightarrow n'}^{(eff)} &= \sum_{l,l'} q_{nl \rightarrow n'l'}^{(eff)} \\ &= \sum_{l,l'} A_{nl \rightarrow n'l'} (N_{nl}^{(z_0-1)} / N_D N^{(z_0)}) \end{aligned} \quad 4.9.3$$

$N_{nl}^{(z_0-1)}$ is the number density of the nl term of the hydrogen-like impurity ion, N_D is the neutral donor number density and $N^{(z_0)}$ is the number density of fully ionised impurity ions. The mean transition energy is

$$\Delta E_{n,n'} = \left(\sum_{l,l'} \Delta E_{n,n'l'} q_{nl \rightarrow n'l'}^{(eff)} \right) / q_{n \rightarrow n'}^{(eff)} \quad 4.9.4$$

where $\Delta E_{nl,n'l'}$ is the line component transition energy and $q_{nl \rightarrow n'l'}^{(eff)}$ is the component effective emission coefficient.

The code first evaluates $q_{n \rightarrow n'}^{(eff)}$ at reference beam/plasma conditions $E_u^{(ref)}$, $N_{zeff}^{(ref)}$, $T_{zeff}^{(ref)}$, $zeff^{(ref)}$ and $B_{mag}^{(ref)}$. Then the $q_{n \rightarrow n'}^{(eff)}$ are obtained at the condition sets

$$\begin{aligned} \{E_{u,i} : i = 1, I_E\}, N_{zeff}^{(ref)}, T_{zeff}^{(ref)}, zeff^{(ref)}, B^{(ref)} & \text{ with } E_u^{(ref)} \in \{E_{u,i} : i = 1, I_E\}, \\ E_u^{(zeff)}, \{N_{zeff} : i = 1, I_N\}, T_{zeff}^{(ref)}, zeff^{(ref)}, B^{(ref)} & \text{ with } N_{zeff}^{(ref)} \in \{N_{zeff} : i = 1, I_N\}, \\ E_u^{(ref)}, N_{zeff}^{(ref)}, \{T_{zeff,i} : i = 1, I_T\}, zeff^{(ref)}, B^{(ref)} & \text{ with } T_{zeff}^{(ref)} \in \{T_{zeff,i} : i = 1, I_T\}, \\ E_u^{(ref)}, N_{zeff}^{(ref)}, T_{zeff}^{(ref)}, \{zeff_i : i = 1, I_{zeff}\}, B^{(ref)} & \text{ with } zeff^{(ref)} \in \{zeff_i : i = 1, I_{zeff}\}, \\ E_u^{(ref)}, N_{zeff}^{(ref)}, T_{zeff}^{(ref)}, zeff^{(ref)}, \{B_i : i = 1, I_B\} & \text{ with } B^{(ref)} \in \{B_i : i = 1, I_B\}, \end{aligned}$$

The results are organised for output directly to the ADF12 specification so that they can be reused interpolatively in other analyses. For widely different plasma conditions from the reference where the rapid interpolation afforded by one dimensional scans is expected to be unsound, it is the practise to set up other ADF12 datasets centred on different reference conditions. The scan densities allowed by the code are larger for beam energy and plasma ion density parameters, since the coefficients are most sensitive to them. The magnetic field scan is not meaningful at this time and a single value is normally entered only for place holding.

Source data :

The program operates on collections of fundamental state selective charge exchange cross-section data. The allowed content, organisation and formatting of these files are specified in ADAS data format ADF01. Centrally supported data collections are stored in directories such as

`../adas/adas/adf01/qcx#h0/`

where the *h0* identifies neutral hydrogen is the donor. The individual data set names take the form

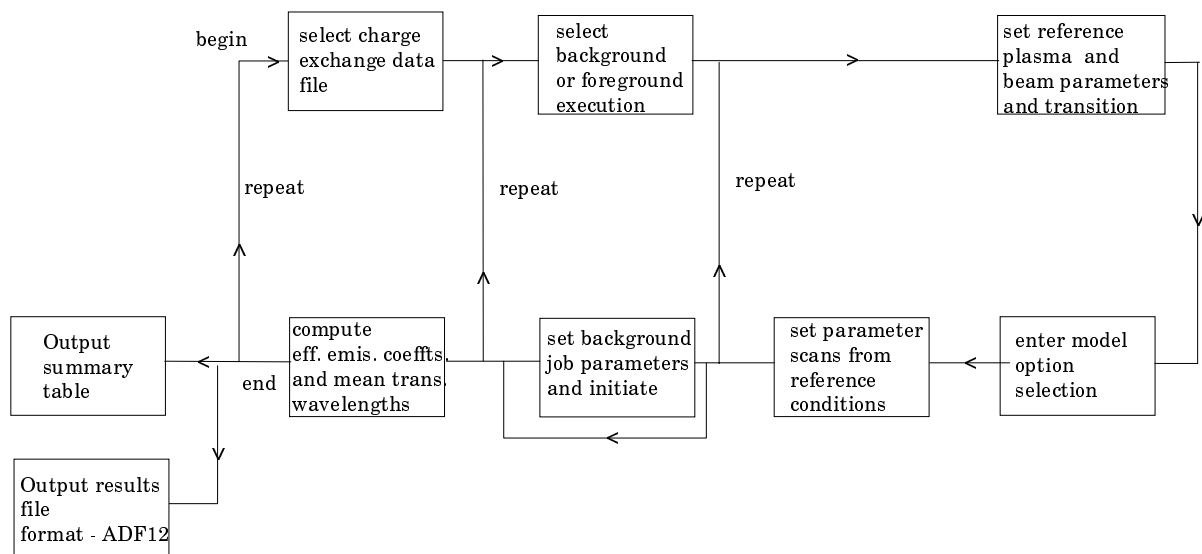
`qcx#h0_<code>.#<ion>.dat`

where *<code>* is a three character identifier of the source and *<ion>* is the receiving fully ionised ion (for example *c6*). More detail is given below.

Program steps:

These are summarised in the figure below.

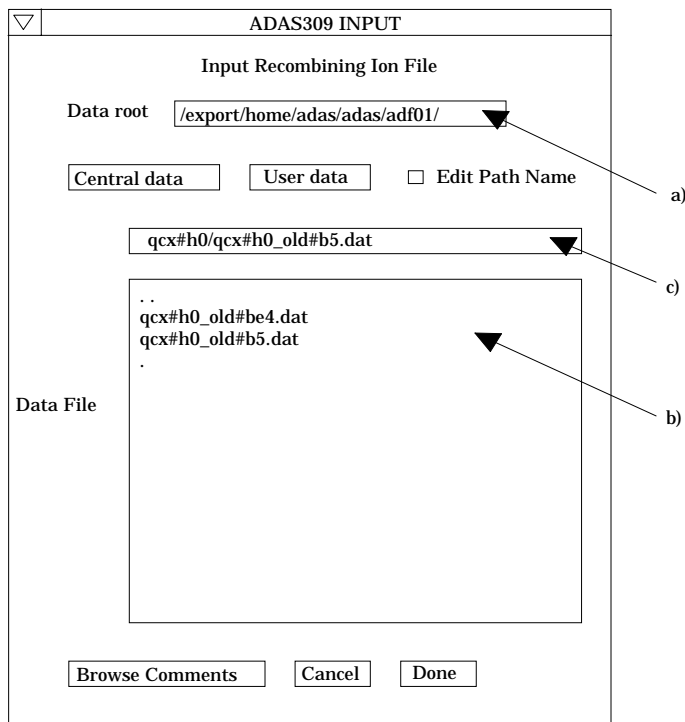
Figure 4.9



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 effective emission coefficient file formatted to adf12 specification. There is no graphic output from this program.

The **file selection window** appears first. Its appearance is as shown below.



1. *adf01* is the appropriate format for use by the program ADAS309. 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 are shown in the large file display window. Scroll bars appear if the number of entries exceed the file display window size. There are a large number of these. They are stored in sub-directories by donor which is usually neutral but not necessarily so (eg. *qcx#h0*). The individual members are identified by the subdirectory name, a code and then fully ionised receiver (eg. *qcx#h0_old#c6.dat*). The data sets generally contain *nl*-resolved cross-section data but *n*-resolved and *nlm*-resolved are handled. Resolution levels must not be mixed in datasets.
3. The codes distinguish different sources. The first letter *o* or the code *old* has been used to indicate that the data has been produced from JET compilations which originally had parametrised *l*-distribution of cross-sections. The *nl*-resolved data with such code has been reconstituted from them. Data of code *old* is the preferred JET data. Other sources codes include *ory* (old Ryufuku), *ool* (old Olson), *ofr* (old Fritsch) and *omo* (old molecular orbital). There are new data such as *kvi*.
4. 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*.
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. 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.
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

ADAS309 : PROCESSING OPTIONS

Title for Run

Data File Name :

Receiver			Neutral donor		
Symbol	Nuclear charge	Initial ion charge	Final ion charge	Symbol	Nuclear charge
B	5	5	4	H	1

Please input the following receiver information

Atomic mass number of receiver

Input reference plasma parameter information :-

Ion temp. (eV) : Elec. temp. (eV) :

Ion dens. (cm-3) : Elec. dens. (cm-3) :

Z effective : B Magn. (T) :

Input reference beam parameter information :-

Beam energy (eV/amu) :

Input selected transition :-

Upper N level Lower N level :

Note : maximum allowed N quantum no. : 20
minimum allowed N quantum no. : 1

Select charge exchange theory

Select donor states

Select emission measure model

Input scan information :-

Beam energy scan

Ion density scan

Ion temperature scan

Plasma effective Z scan

Magnetic induction scan

Beam energy scan

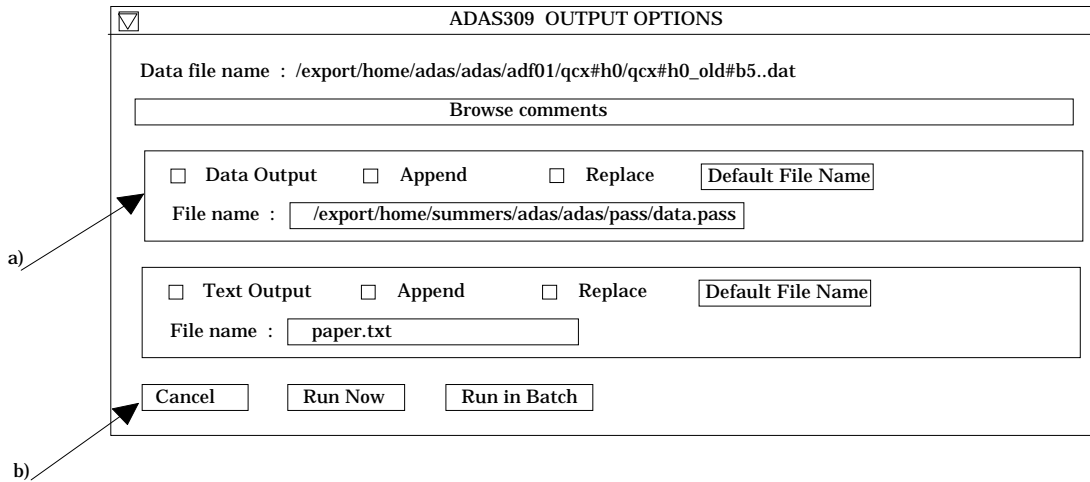
INDEX	Energy (eV/amu)
1	1.000e+04
2	1.500e+04
3	2.000e+04
4	3.000e+04
5	

8. The user input follows broadly that required for ADAS308. The reference plasma parameters are specified at a) with the beam reference energy entered just below. Note that a reference value is usually taken centralised in the one dimensional scan for that parameter. In such one dimensional scans, the other parameters are kept at their reference values. The actual scans are entered by clicking on the appropriate button at b). The selected scan table is displayed at e) and may be edited in the usual manner
9. At c), the particular transition for which the tabulation is to be prepared is entered. This is analogous to ADAS308 but only one transition is treated at a time. At d), the usual model options are available..

The **output options window** is shown below. There is no graphical output possibility but in addition to the usual text file, the data output file may be produced a). It is prepared preformatted according to *adf12* for direct addition to the ADAS database. Since it may be desired to patch the data in to existing *adf12* data sets, the transition count is left blank. More details are given in the ADAS Manual. As the calculations may take some time, the option is given of executing in the background. There are therefore two ways in which output can be generated:

10. By pressing *Run Now* b), 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.
11. By pressing *Run in Batch* the actual calculations required to produce the output are run at a later time, but it is necessary for a batch file containing all relevant data to be created or updated. Again a small information box opens showing the progress made in doing this. The process will normally be considerably quicker than when pressing *Run Now*. A larger batch job can be built up by returning to the Processing Options Window and making new selections before returning to the Output Options Window and again clicking on *Run in Batch*. When you exit the Processing Options Window of ADAS309 by clicking on *Cancel* to return to the Input Options Window, the program takes this as a signal that the batch job is completed and submits it for

execution. A small information box opens giving the name of the job and information on when execution will begin. Calculations run in this way will normally run more quickly than those run using the *Run Now* button. When the batch job is complete, the output files are generated and a mail message sent from the operating system to say that it is finished. This will normally contain a simple message which says 'Your batch job has completed successfully'. It is possible to build a queue of batch jobs by submitting one as described above, constructing another and submitting that in the same way, but due to the relatively short time taken by the calculations it is not anticipated that this will happen very often.



12. Note that care must be taken with filenames when using ADAS309. Whenever the *Replace* option is selected and output then produced, the program automatically deselects the *Replace* option again to prevent the output being accidentally overwritten. When running batch jobs, the program goes one step further. After *Run in Batch* has been selected the first time, the *Append* option is always automatically selected for subsequent output. It is possible to override this and even to send output to different files from the same batch job. However, if the *Replace* button is selected once the construction of a batch file has begun then any earlier output stored in the batch file will be deleted when the job executes.

Illustration:

There is no graphical display from this code.

Table 4.9a.

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ADAS RELEASE: ADAS93 V1.6 PROGRAM: ADAS309 V1.4 DATE: 08/07/96 TIME: 20:31
0*****
***** RUN SUMMARY FOR L-RESOLVED CHARGE EXCHANGE *****
***** EFFECTIVE EMISSIVITY COEFFICIENT SCANNING PROGRAM *****
***** ADAS309 - DATE: 08/07/96 *****

INPUT FILE      : export/home/adas/adas/adf01/qcx#h0/qcx#h0_old#b5.dat
OUTPUT PASSING FILE: home/summers/adas/pass/data3-09.pass

***** SUMMARY OF PARAMETER SET NO. 1 *****

-----
                      cxs-manu
-----

DONOR / RECEIVER INFORMATION:

                RECEIVER          NEUTRAL DONOR
                -----          -----
ELEMENT SYMBOL   =      B          H
NUCLEAR CHARGE  =      5          1
RECOMBINING ION CHARGE =      5          -
RECOMBINED ION CHARGE =      4          -
ATOMIC MASS NUMBER = 11.00          -

PLASMA PARAMETERS:

ION TEMPERATURE (EV) = 5.00D+03      ELECTRON TEMPERATURE (EV) = 5.00D+03
ION DENSITY (CM-3) = 2.50D+13        ELECTRON DENSITY (CM-3) = 5.00D+13
PLASMA EFFECTIVE Z = 2.00            MAGNETIC INDUCTION (T) = 3.00

BEAM PARAMETERS:

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BEAM ENERGY (EV) = 4.00D+04

TRANSITION PARAMETERS:

UPPER N LEVEL = 6    LOWER N LEVEL = 5

CHARGE EXCHANGE MODEL : INPUT DATA SET
EMISSION MEASURE MODEL: CHARGE EXCHANGE

VALUES FOR BEAM ENERGY SCAN:

NUMBER OF BEAM ENERGIES = 8

SET OF BEAM ENERGIES (EV)
  1.00D+04  2.00D+04  3.00D+04  4.00D+04  5.00D+04  6.00D+04
  7.00D+04  8.00D+04

VALUES FOR ION TEMPERATURE SCAN:

NUMBER OF ION TEMPERATURES = 5

SET OF ION TEMPERATURES (EV)
  2.00D+03  3.00D+03  5.00D+03  7.00D+03  1.00D+04

VALUES FOR ION DENSITY SCAN:

NUMBER OF ION DENSITIES = 6

SET OF ION DENSITIES (CM-3)
  1.00D+13  2.00D+13  3.00D+13  5.00D+13  7.00D+13  1.00D+14

VALUES FOR PLASMA EFFECTIVE Z SCAN:

NUMBER OF EFFECTIVE Z = 5

SET OF EFFECTIVE Z
  1.00D+00  2.00D+00  3.00D+00  4.00D+00  5.00D+00

VALUES FOR MAGNETIC INDUCTION SCAN:

NUMBER OF MAGNETIC FIELDS = 1

SET OF MAGNETIC FIELDS (T)
  3.00D+00

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Table 4.9b.

ADAS309 08/07/96 D=H(1S) R= B+5 N= 6-5 F=_old#b5 M=CX						ISEL= 1
4.90D-08						QEFREF
4.00D+04	5.00D+03	2.50D+13	2.00D+00	3.00D+00		PARMREF
	8	5	6	5	1	NPARMSC
						ENER
1.00D+04	2.00D+04	3.00D+04	4.00D+04	5.00D+04	6.00D+04	
7.00D+04	8.00D+04	0.00D+00	0.00D+00	0.00D+00	0.00D+00	
0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	
0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	
1.92D-09	9.38D-09	2.37D-08	4.90D-08	4.92D-08	2.45D-08	QENER
2.10D-08	1.84D-08	0.00D+00	0.00D+00	0.00D+00	0.00D+00	
0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	
0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	
2.00D+03	3.00D+03	5.00D+03	7.00D+03	1.00D+04	0.00D+00	TIEV
0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	
2.71D-08	2.79D-08	4.90D-08	4.97D-08	3.05D-08	0.00D+00	QTIEV
0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	
1.00D+13	2.00D+13	3.00D+13	5.00D+13	7.00D+13	1.00D+14	DENSI
0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	
0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	
0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	
3.39D-08	3.03D-08	2.79D-08	2.49D-08	2.30D-08	2.11D-08	QDENSI
0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	
0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	
0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	
1.00D+00	2.00D+00	3.00D+00	4.00D+00	5.00D+00	0.00D+00	ZEFF
0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	
3.55D-08	4.90D-08	2.46D-08	2.16D-08	1.96D-08	0.00D+00	QZEFF
0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	
3.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	BMAG
0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	
4.90D-08	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	QBMAG
0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	0.00D+00	

Notes: