ADAS202: General z recom/ionis - extraction from general z file

The program extracts radiative recombination, dielectronic recombination and collisional ionisation rate coefficients and associated approximate form parameters for an arbitrary ion of an isoelectronic sequence from a general z recom/ionis. file of type ADF06. It also prepares an input data set for the collisional-radiative code ADAS204 and a partial atomic parameter data set of type ADF03 for the code ADAS408.

Background theory:

Consider a set of members of an isoelectronic sequence of ion charges $\{z_i : i = 1,.., I_s\}$. The z_i are called the *recombined ion charges*. If the nuclear charge of the neutral member of the sequence is z_s, then the member nuclear charges are $\{z_{0,i} = z_i + z_s : i = 1,.., I_s\}$. The *recombining ion charges* are then $\{z_{1,i} = z_i + 1 : i = 1,.., I_s\}$. Data sets of type ADF06 contain parameters of approximate forms for the radiative and dielectronic recombination from the ground state of each recombining ion of the set and ionisation rate coefficients from the ground state of each recombined ion of the set. Additionally, a best available numerical tabulation of each of these coefficients at zero density over a range of *reduced temperatures* $\{\theta_j = T_{e,j} / z_1^2 : j = 1, M\}$ is contained in the dataset. The same set of reduced temperatures applies to the data for each ion of the set. The code interpolates the parameters of the approximate forms to a selected intermediate ion of the sequence. The approximate forms are then used as an interpolation aid to generate numerical values for the coefficients at arbitrary output electron temperatures. In this the code follows closely the approximations and methods described in ADAS103, ADAS104 and ADAS106.

Radiative recombination

The approximate form is

$$\alpha^{approx} = \tfrac{2^7}{3}\sqrt{\tfrac{\pi}{3}}\alpha^4 c a_0^2 z_1 (z_1^2 I_H / kT_e)^{1/2} \{scale (z_1^2 I_H / kT_e \nu_0^2)^{edisp} \frac{2\, phfrac}{\nu_0} (z_1^2 I_H / kT_e \nu_0^2) EEI (z_1^2 I_H / kT_e \nu_0^2) + \sum_{n \geq n_0 + 1} \frac{2}{n} (z_1^2 I_H / kT_e n^2) EEI (z_1^2 I_H / kT_e n^2)\} \qquad 3.2.1$$

being a sum of recombination to the lowest n-shell and to higher n-shells. The recombination to the lowest n-shell , n_0, is modified by including an availability factor *phfrac*, for occupancy for the n-shell and by using an effective principal quantum number ν_0, in the expression. The ground state capture is further adjusted by two external factors *scale* and *edisp* chosen to optimise the approximate form to best available data. More details of these approximate forms are given in the description of ADAS104.

Thus the interpolable parameters are ν_0, *phfrac*, *scale* and *edisp* together with the fixed n_0. Cubic spline interpolation is used with independent variable z_1 and zero curvature end conditions to prepare the parameters for a selected intermediate ion.

For numerical data, the ratios

$$y_{i,j} = y(z_{1,i}, T_{e,j}) = \alpha(z_{1,i}, T_{e,j}) / \alpha^{approx}(z_{1,i}, T_{e,j}) \qquad 3.2.2$$

are formed and interpolated to the selected intermediate z_1 giving the ratios $y_j = y(z_1, T_{e,j})$. The interpolation uses splines with zero curvature end conditions. A second interpolation is conducted in electron temperature with the final recombination coefficient obtained at arbitrary T_e using the approximate form as

$$\alpha(z_1, T_e) = y(z_1, T_e) * \alpha^{approx}(z_1, T_e) \qquad 3.2.3$$

Dielectronic recombination

The approximate form is

$$\alpha^{approx} = \sum_{i \in I} \alpha^{GF}(i; nl) \qquad 3.2.4$$

α^{GP} denotes the algorithm based on the 'General Program' for nl-resolved dielectronic coefficients prepared by Burgess. The sum over nl gives the zero density total coefficient for a particular parent transition. There is one adjustable parameter *corfac* but its precise action depends on details of the quantum numbers of the active core electron in the initial and excited parent. This adjustable parameter is in addition to the parent transition energy and transition probability. The program also allows for termination of the sum through alternative Auger channels of secondary autoionisation by the parameter *ncut* ($\equiv n_S$ or n_C). The complete set of parameters includes parent transition quantum numbers, n_i, l_i, n_j, l_j, transition type , *type*, transition energy, ΔE_{ij}, transition oscillator strength, f_{ij}, Bethe correction factor, *corfac*, the cut-off n-shell, *ncut*, the lowest accessible n shell, n_1 and the parameters for improvement of the General Formula, *scale* and *edisp*. More details of these approximate forms are given in the description of ADAS103. The parameters of both the General Program and General Formula are maintained since this allows production of both the (A) and (B) forms of the atomic parameter data set (see ADAS408). The interpolation procedures parallel exactly those for the radiative recombination coefficient.

Collisional ionisation

The approximate form is

$$S^{approx} = S^{approx}_{shd}(T_e) + S^{approx}_{excit}(T_e) \qquad 3.2.5$$

The shell direct ionisation rate coefficient is

$$S^{approx}_{shd}(T_e) = \sum_I c_I \sum_{i \in I} S^{BCHID}(z, \chi_i, \zeta_i, T_e) \qquad 3.2.6$$

c_I is an adjustable multiplier for the shell group *I*. ζ_i is the number of equivalent electrons for the shell and χ_i the shell ionisation energy.

The excitation-autoionisation rate coefficient is

$$S^{approx}_{excit}(T_e) = \sum_R c_R \sum_{r \in R} 1.45 \tfrac{8\pi}{\sqrt{3}} 2\sqrt{\pi}\alpha c a_0^2 \; WT_r \; (I_H / kT_e)^{1/2} (I_H / \Delta E_r) \exp(-\Delta E_r / kT_e) \qquad 3.2.7$$

where c_R is an adjustable multiplier for the shell group *R*.. WT_r is the weight factor and ΔE_r the effective excitation energy of the resonance. More details of these approximate forms are given in the description of ADAS106. The interpolable parameters are the scalings, c_I, c_R, the number of equivalent electrons ζ_i the shell ionisation energies χ_i the weight factors, WT_r and the excitation energies, ΔE_r. The interpolation procedures follow exactly those for the radiative recombination coefficient.

Program steps:

The code has been discontinued in IDL-ADAS. It remains in IBM-ADAS.

Illustration:

The output from the programme is illustrated for the recombined ion B^{+4}. This hydrogen-like system has no dielectronic recombination. The display graph for the radiative recombination coefficient only is shown. The exact interpolated results are shown as the solid line. The approximate form for the interpolated ion is also displayed as a dotted curve but in this case is superimposed on the exact values.

Figure 3.2a.

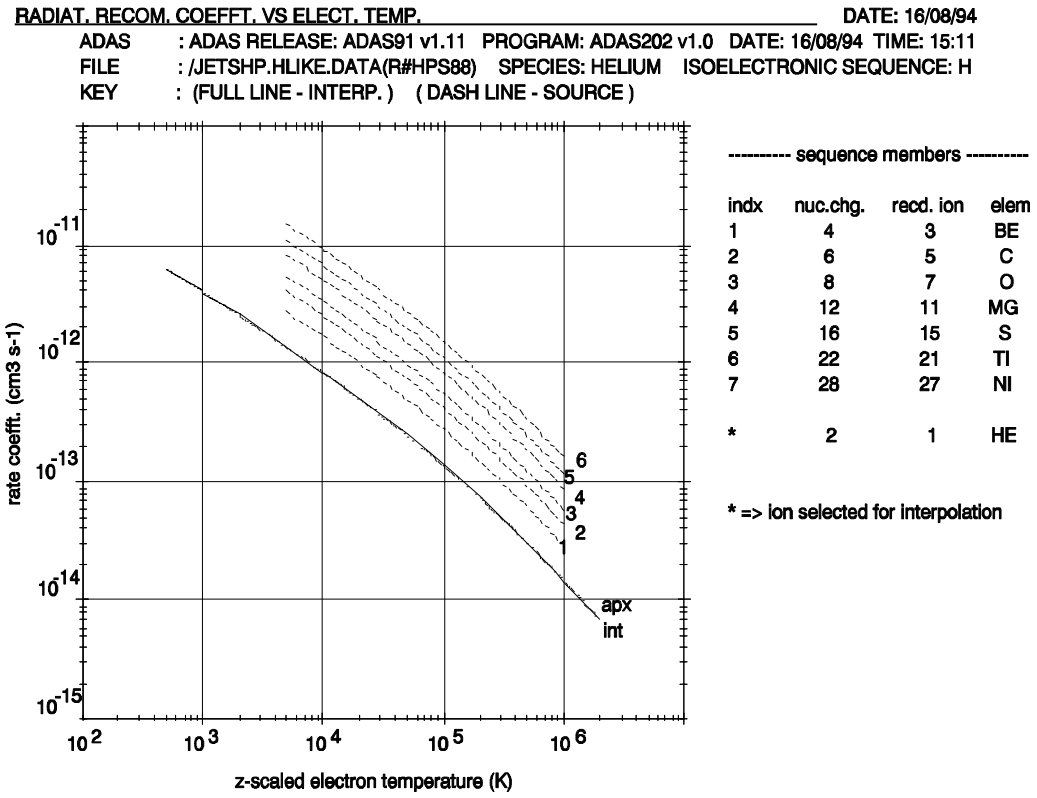

Table 3.2.

```
 ADAS RELEASE: ADAS91 V1.11  PROGRAM: ADAS202 V1.0   DATE: 16/08/94  TIME: 15:12
 ************* TABULAR OUTPUT FROM  GENERAL Z IONIS/RECOM. FILE INTERROGATION PROGRAM: ADAS202 - DATE: 16/08/94
**************

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        RECOM/IONIS. PARMS. AND COEFFTS. AS A FUNCTION OF TEMPERATURE
        ------------------------------------------------------------
                    DATA GENERATED USING PROGRAM: ADAS202
                    ------------------------------------

 FILE: /JETSHP.HLIKE.DATA(R#HPS88)     ELEMENT: ```(Z= 0)

 NUCLEAR CHARGE         (Z0) =   2
 RECOMBINING ION CHARGE (Z1) =   2
 RECOMBINED ION CHARGE  (Z)  =   0


 -------------------------------------------
   REACTION        PROCESS      BAD POINTS
 -------------------------------------------
   RAD.  RECOM.       T              F
   DIEL. RECOM.       F              F
   COLL. IONIS.       T              F


 ---- ELECTRON TEMPERATURES ------  ---------------- RATE COEFFICIENTS (CM3 S-1) ----------------------------------------
    KELVIN      EV     K/Z1**2       RAD. REC.     DIEL. REC.     COLL. ION.     RAD.(APPRX)     DIEL.(APPRX)    ION.(APPRX)
 ---------------------------------------------------------------------------------------------------------------------------
   2.00D+03  1.72D-01  5.00D+02     6.2234D-12     0.0000D+00     0.0000D+00     6.2428D-12      0.0000D+00      0.0000D+00
   4.00D+03  3.45D-01  1.00D+03     3.9858D-12     0.0000D+00     1.3218D-78     3.9983D-12      0.0000D+00      1.3917D-78
   8.00D+03  6.89D-01  2.00D+03     2.5259D-12     0.0000D+00     3.6176D-44     2.5338D-12      0.0000D+00      3.8090D-44
```

```
  2.00D+04  1.72D+00  5.00D+03     1.3550D-12     0.0000D+00     2.1052D-23     1.3592D-12     0.0000D+00     2.2166D-23
  4.00D+04  3.45D+00  1.00D+04     8.3000D-13     0.0000D+00     2.0864D-16     8.3290D-13     0.0000D+00     2.1977D-16
  8.00D+04  6.89D+00  2.00D+04     5.0000D-13     0.0000D+00     7.5851D-13     5.0015D-13     0.0000D+00     7.9349D-13
  2.00D+05  1.72D+01  5.00D+04     2.4650D-13     0.0000D+00     1.2334D-10     2.4487D-13     0.0000D+00     1.2666D-10
  4.00D+05  3.45D+01  1.00D+05     1.3900D-13     0.0000D+00     7.3441D-10     1.3726D-13     0.0000D+00     7.4624D-10
  8.00D+05  6.89D+01  2.00D+05     7.5000D-14     0.0000D+00     1.8692D-09     7.3904D-14     0.0000D+00     1.8769D-09
  2.00D+06  1.72D+02  5.00D+05     3.0600D-14     0.0000D+00     3.2633D-09     3.0471D-14     0.0000D+00     3.2547D-09
  4.00D+06  3.45D+02  1.00D+06     1.4600D-14     0.0000D+00     3.7864D-09     1.4818D-14     0.0000D+00     3.7665D-09
  8.00D+06  6.89D+02  2.00D+06     6.8234D-15     0.0000D+00     3.8435D-09     6.9254D-15     0.0000D+00     3.8233D-09


RADIATIVE RECOMBINATION PARAMETERS
    N0= 1     V0=   1.00000     PHFRAC=   1.00000     EDISP=  -0.05300     SCALE=   0.87000


DIELECTRONIC RECOMBINATION PARAMETERS     NTRANS= 1
            ITRANS    ITYPE N1     V1       PHFRAC    EPSIJ     FIJ      EDISP      SCALE    CORFAC
              1         1    2   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
                           FIT PARAMETERS FOR GP                          0.00000   1.00000


IONISATION COEFFICIENT PARAMETERS     NIGRP= 1     NRGRP= 0
            IIGRP     CI         ZT,EPSI PAIRS
              1     1.069         1  1.00012
```

Notes: