
|SRON| – SPEX

**Ionization and Energy balance in
Collisionally- and Photo-ionized Plasmas**

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**IONIZATION and ENERGY BALANCE in
COLLISIONALLY- and PHOTO-IONIZED PLASMAS**

1 Introduction

The code to calculate the spectra of collisionally-ionized plasma has been applied in many cases, whereas the code for photo-ionized plasmas is still in development. The latter will for example be applicable to the situation in which a gas is irradiated by a strong X-ray source whose spectrum has to be specified.

The *ionization balance* is set up by a balance between ionization and recombination processes (see §2.1. & §2.2.). The subroutine IONCON solves the ionization balance in steady state, whereas SOLCON solves the time-dependent balance for given plasma models.

The *energy balance* determines the temperature structure of the illuminated gas. It is established by a balance between heating and cooling (see §3.1. & 3.2.). The subroutine BALANCE calculates the total net heating and cooling rate due to all different processes with the rates in W/m³. In the subroutine CONSTART there is an algorithm for finding those parameters for which the heating balances exactly the cooling. The equation to be solved is generally very non-linear. In the case of photo-ionization one might think to start with a source with a prescribed physical parameter which either may be the temperature, the density, or the total pressure.

2 Ionization balance

In a *steady state* the ionization balance is solved in the subroutine IONCON according to the equation:

$$0 = \frac{dn_j}{dt} = \sum_{k=1}^{j-1} S_{j-k,k} n_k - \sum_{i=j+1}^N S_{ij} n_j - \alpha_j n_j + \alpha_{j+1} n_{j+1}, \quad (1)$$

where j is the index of the particular ionization stage considered, i and k are summation indices, N is the maximum ionization stage present (the atomic number + 1), n_j is the relative concentration of ion j , S_{ij} is the ionization rate for ion j with ejection of i electrons, and α_j is the recombination rate of ion j . The first term represents gains from ionizations of less charged ions, the second term represents ionization losses to higher charged ions, the third term represents recombination losses and the fourth term represents recombination gains. Equation (1) is valid as far as the quantities are defined (i.e. the index i should always be less or equal to the maximum numbers of electrons ejected by one ionization, parameter NAUG which is currently 10).

Since neutral atoms can neither recombine further nor be formed by ionization of less charged ions, equation (1) for $j = 1$ simplifies to

$$0 = \frac{dn_1}{dt} = - \sum_{i=2}^N S_{i1} n_1 + \alpha_2 n_2, \quad (2)$$

From (2), the ratio n_2/n_1 can be estimated. The equation for $j = 2$ involves only n_1 , n_2 and n_3 , hence it can be used to calculate n_3 for given n_1 and the solution of (2). Using this recursive algorithm, all concentrations can be expressed in terms of n_1 . Finally, by normalising the sum of the concentrations to 1, n_1 can be determined.

The subroutine CONDEC determines whether the loop for the determination of the ion concentrations can be finished. If the energy balance is in equilibrium the programme continues with the next step, else it goes back to CONSTART which is the driving routine for the determination of the ion concentrations.

In a time-dependent (transient) state the left-hand member of eq. 1 cannot be put to zero. In that case the ionization balance is solved according to the method of Kaastra and Jansen (1993) in the routine SOLCON, but now with an improvement by interpolation.

The calculation is done with double precision (this is required because of round-off problems for elements with many ionization stages). Because the data file containing the required matrices etc. is so large, we only read the data for a narrowed temperature range, and put this into a memory buffer. As soon as the calculation attains temperature values outside this initial range, a new buffer is read (either below or above the old temperature range, depending upon which side the original temperature range is left).

At each timestep, the old concentrations serve as the starting values for the new concentrations. Contrary to Kaastra and Jansen, we do not round-off the temperatures to the grid-values, but merely interpolate as described in timehist. Therefore at each time step we advance the solution using 2 grid temperatures, and interpolate the resulting concentrations using the pre-calculated weights w . This should give more accurate values than calculated by Kaastra and Jansen. On the other hand, we use a grid with a spacing twice as large; this is because we include now more chemical elements, which increases the size of the data files by more than a factor of 3.

2.1 Ionization processes

The ionization rate is composed of several contributions:

1. direct electron collisional ionization (subroutine ELEION)
2. electron excitation-autoionization (ELEION)
3. photo-ionization (FOTION)
4. Compton ionization (COMION, currently dummy)
5. charge-transfer ionization (CHEION)
6. Auger ionization (AUGDIS)

2.1.1 Direct ionization and autoionization

These processes are calculated per subshell of an ion in routine ELEION. Currently we use there the code of Arnaud and Rothenflug (1985) (AR) (which is only applicable for 14 elements; in the future we will calculate rate coefficients for all elements with atomic number $Z \leq 30$). This subroutine calls the old IONIS subroutine (called here IONISAR and included in the fortran code explicitly). A new subroutine valid for all elements has to be constructed. As an additional option for the special case of the ionization equilibrium balance of iron we can use the ion concentrations calculated by Arnaud and Raymond (1992). Since AR do not define the rate for H in their code (but they do in their paper) we modified the old FILE_IONIS program to include H. We express all rates in units of 10^{-20} m³/s (contrary to AR, which use units of cm³/s = 10^{-6} m³/s). Also, we currently act as if all ionizations take place in the outermost shell (which is not actually the case). The energy lost by the free electrons per ionization is simply I , the ionization potential of the subshell considered.

2.1.2 Photo-ionization

The rate S of photo-ionization is calculated by the routine FOTION which convolves the incoming radiation field with the photo-ionization cross sections of all electron shells of all relevant ions. The rate is expressed in processes/s/ion. The convolution is also done to compute the corresponding heating by photo-electrons ϵ (keV/s/ion) (Auger electrons excluded here).

The rates are calculated with the following formulae:

$$S = \int_I^\infty \sigma_{\text{ph}}(E)F(E)dE, \quad (3)$$

$$\epsilon = \int_I^\infty \sigma_{\text{ph}}(E)F(E)(E - I)dE = \int_I^\infty \sigma_{\text{ph}}(E)F(E)EdE - SI, \quad (4)$$

where E is the photon energy (keV), I the ionization potential of the shell (keV), $F(E)$ is the incoming photon spectrum (in 10^{28} photons/s/keV/m²) and $\sigma_{\text{ph}}(E)$ is the photo-ionization cross section for the shell (in barn; 1 barn = 10^{-28} m²). The latter cross section is calculated (added over all shells of all ions) by SIGFOT according to:

$$\sigma_{\text{ph}}(E) = \sum_{ik} C_i \sigma_{ik}(E), \quad (5)$$

where $\sigma_{\text{ph}}(E)$ is the total photo-ionization cross section, the index i denotes all possible ions and the index k denotes all possible shells of ion i ; C_i is the concentration of ion i with respect to Hydrogen, and $\sigma_{ik}(E)$ is the cross section for shell k of ion i .

The integrals in eqs. 3 and 4 are evaluated by calculating the sum (for S ; similar for ϵ)

$$S = \sum_i \sigma(E_i) \times [F(E_i)dE_i]. \quad (6)$$

Since the σ -values are stored on a logarithmic energy grid, we input for efficiency reasons not the energy grid E_i but $^{10} \log E_i$. Also not the spectrum $F(E_i)$ but the product $F(E_i)dE_i$ is inputted for efficiency reasons. Efficiency is very important for this subroutine, since for a full calculation all 2167 shells should be convolved with an energy spectrum of several hundreds of bins.

The σ -values are calculated as follows. We interpolate them linearly on a $\log E$ - $\log \sigma$ grid. For high photon energies outside the grid, we extrapolate using the last two grid points. The logs of the cross sections on the energy grid are stored in the integer*2 array JFOT. For each of the 2167 possible shells, JFOT has 128 entries; the first entry is $10^4 I$ with I in keV; the next 127 entries contain the quantity $3600^{10} \log \sigma$ with σ in barns (the units and multiplication constants are chosen in order to span the complete relevant range with retaining sufficient significant digits). Finally the energy grid for each shell is different: the first 21 points have a spacing of 0.01 in $\log E$ from $\log I$ to $0.20 + \log I$, the next points have a spacing of 0.02 in $\log E$ up to $0.78 + \log I$, and then a spacing of 0.06 in $\log E$ up to $5.40 + \log I$ follows. This grid is chosen in such a way as to describe accurately (within a few percent) the variations of the cross section, in particular near Cooper minima and maxima close to the ionization edge.

2.1.3 Compton ionization

The subroutine COMION (currently a DUMMY routine) calculates the Compton ionization rate S by convolving the incoming radiation field with the Compton ionization cross sections of all electron shells of the relevant ions. The rate is in processes/s/ion. The convolution also serves to calculate the corresponding heating by photo electrons ϵ (keV/s/ion) (Auger electrons excluded here).

In IONIS1 the photo-ionization rate (S_{ph} , from subroutine FOTION) and the Compton-ionization rate (S_C , from subroutine COMION) are added to the total photon-induced ionization rate S_{phi} :

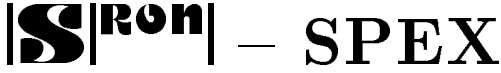
$$S_{phi} = S_{ph} + S_C \quad (7)$$

where all rates are in units of ionizations/s/ion.

Finally, in IONIS2 the photon-induced ionization rate S_{phi} (from IONIS1) and the electron ionization rate S_e (from ELEION) are added to the total ionization rate S_t (exception: charge transfer reactions):

$$S_t = S_{phi} + n_e S_e, \quad (8)$$

where S_{phi} and S_t are in units of ionizations/s/ion, n_e is in units of 10^{20} m^{-3} and S_e is in units of $10^{-20} \text{ ionizations m}^3/\text{s/ion}$.

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2.1.4 Charge-transfer ionization

Charge-transfer ionization rates for given temperature are calculated in CHEION. These are reactions of the type:



where X is an arbitrary chemical element.

We use the formulae and parameters as given by Arnaud and Rothenflug (1985) (AR) in table IIIB. The rates are calculated using 2 different formulae:

$$R(T) = ae^{-d/t}(1 - 0.93e^{-cT}), \quad (11a)$$

$$R(T) = ae^{-d/t}T^b e^{-cT}, \quad (11b)$$

where a,b,c, and d are constants given by AR (we changed them to adjust to the units used in the present work, i.e. T in keV etc.), and $R(T)$ is the ionization rate per ion and per H/He ion. Formulae (11a) and (11b) apply only for

$$T_{\min} < T < T_{\max}, \quad (12)$$

with the limits given by AR (they are different for each reaction). Outside this temperature range the process can be neglected. The ionization rate for ion X is now given by (units ionizations/s/ion)

$$S(X) = R(T)C(Y)n_{\text{H}}, \quad (13)$$

where Y is either H^+ or He^+ and $C(Y)$ is the concentration of Y. This ionization process implies recombination for Y, the recombination rate is given by

$$\alpha(Y) = R(T)C(X)n_{\text{H}}. \quad (14)$$

In the subroutine IONREC3 are the charge-transfer ionization (or recombination) rates added to the other ionization (or recombination) rates in order to obtain the total ionization rate S (or recombination rate α). Note that for the first call, or for runs without charge exchange (in both cases ICEDEC

= 0) the charge exchange rates are *not* added, because in the iteration loop we start with calculating the concentrations without the effect of charge exchange.

Finally, a few remarks about the calculation of the charge-transfer processes.

CESTART is the driving routine for the determination of the ion concentrations subpart which includes charge-transfer reactions. It starts the calculation of the charge-exchange correction on the ionization balance (or continues the iteration at the following step), using some initial guess of the ion concentration. For the first time the ion concentrations are from SETCON, and at the next steps from IONCON. The loop is closed at module CEDEC.

The routine CEDEC determines whether the loop over the charge-transfer reactions can be finished, i.e., whether the calculated ion concentrations are close enough to the start concentrations from CESTART. If the answer is NO then the programme jumps back to CESTART with new input from IONCON, else it continues with COMHEAT.

The criterion used is that all variations in the relative abundances of the ions (relative compared to the elemental abundance) are smaller than a certain number (parameter CEDIFMAX).

If all the differences are small indeed, the loop is closed, otherwise the currently calculated relative concentrations C_c replace the old relative concentrations C_o according to formula (15) below, and in the next iteration new concentrations will be calculated using C_s as starting guess.

$$C_s = 0.9C_c + 0.1C_o. \quad (15)$$

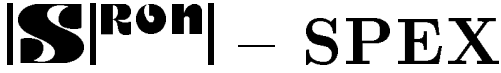
We use the factors 0.9 and 0.1 instead of the values 1 and 0 which appear to be more natural at a first glance. However it appears that sometimes a particular ion concentration switches between 2 different values (e.g. for $T=0.007$ keV many iterations were required in collisional equilibrium (over 20000); by taking the choice (15) the number of iterations for $T=0.007$ keV reduces to 59. This temperature is probably a "worst case". The price paid by the choice (15) is that in cases of high temperatures, where charge-transfer processes are insignificant, 5 iteration steps are required instead of 2.

2.1.5 Auger ionization

In AUGDIS we calculate the distribution of the number of electrons liberated during one primary (inner shell) ionization by Auger processes, multiplied by the ionization rate itself; it also calculates the heating rate per ion due to Auger electrons. So it calculates the probability distribution for multiple ionization. The algorithm is:

$$S(i) = \sum_j p(i, j) S_s(j), \quad (16)$$

where $S_s(j)$ is the total ionization rate in units of ionizations/s/ion for subshell j of the ion, $p(i, j)$ is the probability that an ionization of subshell j leads to a total number of i ejected electrons, and

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$S(i)$ is the required transition rate, the total number of ionizations with i electrons liberated per unit time and per ion, in the same units as $S_s(j)$ (cf. Kaastra and Mewe 1993).

2.2 Recombination processes

The recombination rate is composed of the contributions:

1. radiative recombination (subroutine RECOMB)
2. dielectronic recombination (RECOMB)
3. charge-transfer recombination (CHEREC)

2.2.1 Radiative and dielectronic recombination

The subroutine RECOMB calculates the total recombination (radiative plus dielectronic) rate per level and per ion, summing up over all excited levels. Currently we use Arnaud and Rothenflug (1985) (AR) (only valid for 14 elements). This subroutine calls the old RECOMB subroutine (called here ARRECOMB and included in the fortran code explicitly). A new subroutine valid for all elements has to be constructed.

We express all rates in units of 10^{-20} m³/s (contrary to AR, which use units of cm³/s = 10^{-6} m³/s).

The energy lost by the free electrons per recombination is following Kallman and McCray (1982) $0.75kT$. This is a very crude ad hoc assumption and has to be improved by direct calculation of the energy loss in future.

2.2.2 Charge-transfer recombination

The charge-transfer recombination rates for given temperature are calculated in CHEREC. These are reactions of the type:



where X is an arbitrary chemical element.

We use the formulae and parameters as given by Arnaud and Rothenflug (1985) (AR) in table IIIA. The rates are calculated using the following formula:

$$R(T) = aT^b(1 + ce^{dT}), \quad (19)$$

where a,b,c, and d are constants given by AR (we changed them to adjust to the units used in the present work, i.e. T in keV etc.), and $R(T)$ is the ionization rate per ion and per H/He ion. Formula (19) applies only for

$$T_{\min} < T < T_{\max}, \quad (20)$$

with the limits given by AR (they are different for each reaction). Outside this temperature range the process can be neglected. The recombination rate for ion X is now given by (units recombinations/s/ion)

$$\alpha(X) = R(T)C(Y)n_H, \quad (21)$$

where Y is either H I or He I and $C(Y)$ is the concentration of Y. This ionization process implies ionization for Y, the ionization rate is given by

$$S(Y) = R(T)C(X)n_H. \quad (22)$$

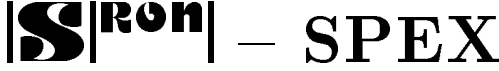
The charge-transfer processes are added to the other recombination processes again in routine ION-REC3 (see above).

3 Energy balance

3.1 Heating processes

The heating occurs by the following processes:

1. photo-ionization (subroutine PIHEAT)
2. Compton ionization (CIHEAT)
3. Compton heating (COMHEAT)
4. free-free absorption (FFHEAT)
5. heating by Auger electrons (AUGHEAT)
6. collisional de-excitation (DEXHEAT, currently dummy)
7. charge transfer

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3.1.1 Photo-ionization

PIHEAT calculates the heating due to the photo-electrons (in W/m³). The rate is calculated with the following formula:

$$H_p = kn_H \sum_{ijk} C_{ij} \epsilon_{ijk}, \quad (23)$$

where i denotes the atomic number, j the ionization stage, k the shell number, C_{ij} the ion concentration with respect to Hydrogen, n_H the Hydrogen density in units of 10²⁰ m⁻³ and ϵ_{ijk} are the heating rates per shell (in keV/s/ion) as calculated by subroutine FOTION (see §2.1.3.). Finally k is a conversion constant to obtain W/m³; it is equal to 10²⁰ × 1 keV (all in SI units), i.e. 1.60217733 × 10⁴.

3.1.2 Compton ionization

CIHEAT calculates the heating due to the photo-electrons generated by Compton-ionization (in W/m³). The rate is calculated with the following formula:

$$H_c = kn_H \sum_{ijk} C_{ij} \epsilon_{ijk}, \quad (24)$$

where i denotes the atomic number, j the ionization stage, k the shell number, C_{ij} the ion concentration with respect to Hydrogen, n_H the Hydrogen density in units of 10²⁰ m⁻³ and ϵ_{ijk} are the heating rates per shell (in keV/s/ion) as calculated by subroutine COMION (see §2.1.4.). Finally k is a conversion constant to obtain W/m³; it is equal to 10²⁰ × 1 keV (all in SI units), i.e. 1.60217733 × 10⁴.

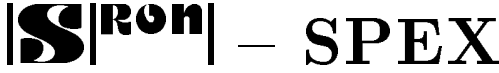
3.1.3 Compton heating

COMHEAT calculates the heating and cooling by Compton scattering of the incoming radiation field with the electrons. We use the formulae as given by Ferland and Rees (1988) (FR), with the following modifications: The heating rate H_C (units W/m³) is written as

$$H_C = \frac{n_e}{m_e c^2} \int \sigma_h E^2 F(E) \{1 + \eta_E [1 - e^{-E/kT}]\} dE, \quad (25)$$

while for the cooling rate C_C (units W/m³) we write

$$C_C = \frac{n_e}{m_e c^2} 4kT \int \sigma_c E F(E) dE, \quad (26)$$

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where E is the photon energy, T the electron temperature, $F(E)$ the incoming photon spectrum (in units of photons/s/m²/keV) and $\sigma_h \equiv \sigma_T \alpha$ and $\sigma_c \equiv \sigma_T \alpha \beta$ are effective cross sections as defined by FR. Here σ_T is the Thomson cross section, and α and β are defined in equation (14) and (15) of FR. We converted the constants there from Rydberg to keV units, leading to the following expressions:

$$\alpha = \frac{1}{1 + E(a + bE)} \quad (27)$$

$$\beta = 1 - \alpha E(a/4 + bE/2), \quad (28)$$

where $a = 8.667 \times 10^{-3}$ keV⁻¹ and $b = 5.207 \times 10^{-8}$ keV⁻¹.

If the electron density is expressed in units of 10²⁰ m⁻³, the photon spectrum in 10⁻²⁸ photons/s/m²/keV, energies and temperatures in keV as throughout this work, the numerical fore-factor of (25) and (26) is 20.858009 (i.e. the product of 10²⁸, 10²⁰, σ_T (m²), 1 keV in J, divided by the electron rest mass energy (in keV)).

Finally, the factor η_E is a dimensionless correction factor for induced Compton heating minus stimulated cooling; it is given by (cf. Levich and Sunyaev 1970):

$$\eta_E = \frac{c^2 h^3 F}{8\pi E^2}. \quad (29)$$

In our units used before we may write the numerical constant in (29) as 2.5295248×10^{-9} (i.e. the product of $c^2 h^3$ in SI units divided by 8π and by (1 keV in J)³).

The integration is performed using simple binwise multiplication and addition.

3.1.4 Free-free absorption

FFHEAT calculates the heating rate due to free-free absorption.

If the Hydrogen density n_H is expressed in units of 10²⁰ m⁻³, the incoming photon spectrum $F(E)$ in units of 10²⁸ photons/s/m²/keV, energies in keV and the free-free absorption cross sections σ_{ff} in 10⁻²⁸ m² as throughout this work, the heating rate due to free-free absorption in W/m³ is given by (cf. Ferland and Rees 1988):

$$H_{ff} = k \int_0^\infty \sigma_{ff}(E) F(E) E dE, \quad (30)$$

where the constant $k = 1.60217733 \times 10^4$. The integration is performed using simple binwise multiplication and addition. The total free-free Gaunt absorption cross section σ_{ff} per Hydrogen atom

is calculated in ABSFF as a function of energy for the plasma (with Kirchhoff's law and the earlier calculated Gaunt factor (in GAUNTFF, see document about continuum radiation processes).

The algorithm is simply applying Kirchhoff's law, see e.g. Rybicki and Lightman (1979), p. 162. We may write it in the following form:

$$\sigma_{\text{ff}} = 7.667025 \times 10^{-10} \frac{(1 - e^{-E/T}) n_e G_{\text{ff}}}{E^3 \sqrt{T}}, \quad (31)$$

where σ_{ff} is the free-free absorption coefficient per Hydrogen atom in barn (10^{-28} m^2), E and T are the photon energy and electron temperature, both in keV, n_e is the electron density in units of 10^{20} m^{-3} and G_{ff} is the total Gaunt factor for bremsstrahlung as calculated by subroutine GFF.

The constant in this equation is given by

$$\frac{\sqrt{2m_e} \alpha \sigma_T c^4 h^3}{4\pi \sqrt{3\pi} (1\text{keV})^{7/2}}, \quad (32)$$

where all quantities are in SI units (α is the fine-structure constant).

3.1.5 Auger heating

AUGHEAT calculates the total heating due to the Auger electrons (in W/m^3). The rate is calculated with the following formula:

$$H_A = k n_H \sum_{ij} C_{ij} \epsilon_{ij}, \quad (33)$$

where i denotes the atomic number, j the ionization stage, C_{ij} the ion concentration with respect to Hydrogen, n_H the Hydrogen density in units of 10^{20} m^{-3} and ϵ_{ij} is the heating rate per ion (in keV/s/ion) as calculated by subroutine AUGDIS (see §2.1.6.). Finally k is a conversion constant to obtain W/m^3 ; it is equal to $10^{20} \times 1 \text{ keV}$ (all in SI units), i.e. 1.60217733×10^4 .

3.1.6 De-excitation

The subroutine DEXHEAT (which is currently a DUMMY routine) will calculate the heating due to collisional de-excitation.

3.1.7 Charge-transfer

No routine currently available.

3.2 Cooling processes

The cooling occurs by:

1. radiative recombination (RECCOOL)
2. dielectronic recombination (RECCOOL)
3. bremsstrahlung (inverse Compton cooling) (COMHEAT)
4. free-free emission (FFCOOL)
5. collisional ionization (IONCOOL)
6. collisional excitation of bound levels (EXCOOL, currently dummy)
7. charge transfer

3.2.1 Radiative and dielectronic recombination

RECCOOL calculates the cooling rate due to recombinations C_R for the plasma. Note that charge-exchange ionization and recombination yields no direct energy gain for the free electrons because no free electrons are involved in these processes.

$$C_R = n_e n_H \sum_{ij} c_{ij} \epsilon_{ij}, \quad (34)$$

where i denotes the atomic number, j the ionization stage. c_{ij} is the concentration (with respect to Hydrogen) of the ion, and the ϵ_{ij} represent the energy per unit of time per ion lost by ionizations (calculated by subroutine RECCOMB, see §2.2.1).

3.2.2 Inverse Compton cooling

The cooling is calculated in subroutine COMHEAT (cf. §3.2.3).

3.2.3 Free-free emission

FFCOOL calculates the cooling rate due to free-free emission. If the Hydrogen density n_{H} and electron density n_e are expressed in units of 10^{20} m^{-3} , the cooling rate due to free-free emission in W/m^3 is given by

$$C_{\text{ff}} = k n_e n_{\text{H}} G_{\text{ff}} \sqrt{T}, \quad (35)$$

where the constant $k = 4856.222$ is (compare Carson 1988):

$$\frac{10^{20} 10^{20} 16(2\pi)^{3/2} e^6 (1\text{keV})^{1/2}}{(3m_e)^{3/2} (4\pi\epsilon_0)^3 h^3 c^3}, \quad (36)$$

and G_{ff} is the total free-free Gaunt factor calculated by GAUNTFF (see document on continuum radiation).

3.2.4 Collisional ionization

IONCOOL calculates the direct-ionization plus excitation-autoionization cooling rate C_I for the plasma:

$$C_I = n_e n_{\text{H}} \sum_{ij k} c_{ij} \epsilon_{ijk}, \quad (37)$$

where i denotes the atomic number, j the ionization stage and k the shell number; c_{ij} is the concentration (with respect to Hydrogen) of the ion, and the ϵ_{ijk} represent the energy per unit of time per ion lost by ionizations (calculated by subroutine ELEION (see §2.1.1)).

3.2.5 Collisional excitation

EXCOOL (currently a DUMMY routine) will calculate the cooling due to collisional excitation.

3.2.6 Charge transfer

No routine currently available.

4 Total continuum absorption

In non-optically thin models one must calculate the attenuation of the incident radiation which traverses the plasma. In the case of continuum absorption the subroutine ABSCON adds the photoionization cross section (as calculated by SIGFOT, see §2.1.3.) and the free-free absorption cross section (as calculated by ABSFF, see §3.2.4.) to the total continuum absorption cross section:

$$\sigma_t = \sigma_{\text{ph}} + \sigma_{\text{ff}}. \quad (38)$$

For example, in the simple case of a homogeneous plasma slab of thickness D the total column density would be $\sigma_t \times D$.

5 References

Arnaud, M., Rothenflug, R.: 1985, *Astron. Astrophys. Suppl.* **60**, 425

Arnaud, M., Raymond, J.C.: 1992, *Astrophys. J.* **398**, 394

Carson, T.R.: 1988, *Astron. Astrophys.* **189**, 319

Ferland, G.J., Rees, M.J.: 1988, *Astrophys. J.* **332**, 141

Kaastra, J.S., Jansen, F.A.: 1993, *Astron. Astrophys. Suppl.* **97**, 873

Kaastra, J.S., Mewe, R.: 1993, *Astron. Astrophys. Suppl.* **97**, 443

Kallman, T.R., McCray, R.: 1982, *Astrophys. J. Suppl. Series* **50**, 263

Kylafis, N.D., Lamb, D.Q.: 1982, *Astrophys. J. Suppl. Series* **48**, 239

Levich, E.V., Sunyaev, R.A.: 1970, *Astrophys. Letters* **7**, 69

Rybicki, G.B., Lightman, A.P.: 1979, *Radiative processes in astrophysics*, Wiley, New York