SRON – SPEX

Line Excitation Processes

SRON/SPEX/TRPB04

Version 1.0/Rev. 2.0

August 25, 1994

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LINE EXCITATION PROCESSES (subroutine linem)

1 Introduction

In the subroutine LINEM the line emissivities in an optically thin plasma are calculated. In this document the various contributing processes are shortly described and all formulae used in LINEM are treated.

2 Algorithm

The algorithm calculates the individual line emissivities for all lines included in a data file 'PARLIN' which is converted from the original line data input file LINEPAR.ASC which is written in ASCII-format and which contains many atomic parameters. LINEPAR.ASC is described below. The lines are calculated within two loops: an outer loop over all elements, and an inner loop over all ions for each element. For each line, there are 5 possible emission mechanisms (in the future additional processes, viz. photo-excitation and charge-transfer processes will be added to this list in the case of photo-ionized plasmas) (initiated by flags ERDSIPC set to nonzero in 'LINEPAR.ASC'):

For each line, the emissivity due to each of these processes (if relevant) is calculated separately. If the emissivity is positive, the line is added to a list of relevant lines. There is a possibility to add all contributing processes first before a new line is added to the output list.

The algorithm for each line consists of two steps: in the first step, the emissivity due to each contributing process is calculated in the zero electron density limit; in the next step, a density correction is applied (flag 'N') (cf. §3.) and lines which are coupled ('mixed', flag 'M'; currently only for the He-like forbidden and intercombination lines) (cf. §4.) are also calculated.

Currently the line data are based upon the latest version of the Utrecht line list, including 5150 lines of a restricted set of 16 elements. This set is an update of the list of paper V, with more than 1000 dielectronic recombination (DR) satellites and 400 Kα and Kβ lines (between 1–42 Å) added, plus several about 300 UV lines (in the wavelength region 300–2000 Å) from a list of Landini and Monsignori-Fossi. A major revision of the atomic data parameters and line wavelengths is in progress. Now (date: 28 April 1993) we have finished the H I- up to the B I-isoelectronic sequence.

2.1 Description of the line parameter data file LINEPAR.ASC

The parameter file contains 26 columns and 9 flags ERDSIPCMN which are set nonzero if the corresponding process is active (E = excitation, R = radiative recombination, etc, see above). We give some examples for explanation.

The first eight columns are:

(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)
LNUM	Z	EL	IO	IE	SN	TRANS	LAMBDA
1876	26	Fe	22	5	0	B2A DE	8.96000
1877	26	Fe	21	6	0	B2A*	8.96000
1878	26	Fe	22	5	0	B2B1	8.96000
69	28	Ni	27	2	2	HE J	1.54170

The first column is the line number, the second the atomic number Z, the third the element letter notation, the fourth the ionization stage (1=neutral atom, 2=first ion, etc.; e.g. Fe 22=Fe XXII=$Fe^{+21}\equiv Z^{+z}$ with Z=26 and z=IO–1=21); 5th column: IE=Z–IO+1=nr. of iso-el. sequence (e.g. IE=1,2,3 for H I, He I, Li I seq., respectively); 6th column indicates a satellite line with principal quantum number n for the 'spectator' electron (e.g. SN=2 is a n=2 satellite); the 7th column gives the transition (e.g. B2A indicates line 2A in the B I isoelectronic sequence, DE = density-sensitive line; B2A* : the asterisk indicates a close 'unresolved' satellite to the resonance line B2A); 8th column: line wavelength λ in Å. We note that TRANS is not used in the program but is given only for additional information in the ascii parameter file. Columns 9–19:

(9)	(10)	(11)	(12)	(13)	(14)	(15)	(16)	(17)	(18)	(19)
F'	F	BR	CC	aEX	aDR	A	B	C	D	E
0.08790	0.10650	0.8250	1.000	1.000	0.000	0.000	0.222	0.000	0.0000	0.276
0.00000	0.00000	0.0000	1.000	1.000	0.700	0.000	0.000	0.000	0.0000	0.000

The columns contain: the corrected oscillator strength f', the absorption oscillator strength f_{ij}, the branching ratio B, the cascade correction C, the ratio $a_{\rm EX}$ = excitation energy/line energy (= 1 for resonance and > 1 for non-resonance transitions), and the corresponding ratio a_{DR} for DR satellites (< 1 in this case). Finally, the last five columns give the excitation Gaunt factor parameters A, B, etc. The excitation parameters are described in §2.2.

Columns 20–26:

(20)	(21)	(22)	(23)	(24)	(25)	(26)
AREC	ETA	CDR	CII	ALPHA	BETA	GAM
00.0000	0.000	0.0000	0.0000	000.000	00.000	0.00

These columns contain: parameters $AREC$ and η in the formula for radiative recombination (§2.3.), $C_{\rm DR}$ for dielectronic recombination (§2.5.), and $C_{\rm II}$ the branching ratio for innershell ionization (§2.6). Finally, the parameters α, β, and γ are used in formulae describing the density corrections (§3).

Finally, there are nine additional columns that contain the flags:

E	R	D	S	I	P	C	M	N
1	1	0	0	0	0	0	0	3
0	0	0	2	0	0	0	0	0
0	0	0	1	0	0	0	0	0
1	0	0	1	0	0	0	0	0
0	0	0	1	0	0	0	0	1
1	1	0	0	1	0	0	3	1

The first line belongs to a spectral line that has a contribution from collisional excitation (E = 1) and radiative recombination (R = 1), and that has a density dependence (N = 3). In the latter case the density flag N is at the same time used to indicate the type of correction formula (e.g. here eq. 35.3 in §3.2.). The second line refers to an 'unresolved' (from the main resonance line) dielectronic recombination (DR) satellite (S = 2), the third line to a DR satellite (S = 1), the 4th line to a DR satellite which also contains a contribution from innershell excitation (E = 1). The fifth line is a spectral line which is a DR satellite line that has a density dependence described by formula (35.1) (N = 1) (cf. §3.1.). The last line in the example refers to a forbidden He-like line (He z) which contains contributions from excitation, recombination (in this case including also dielectronic recombination, cf. §2.4.), innershell ionization (I = 1), mixing (= coupling) with the intercombination lines x and y (notation x, etc. from Gabriel (1972)). The mixing flag M = 1, 2, and 3 for x, y, and z, respectively, cf. §4.). Finally, we remark that though the He-like z line has also a density correction (N=1) which is approximately described by eq. 35.1 of §3.1., we can better apply the mixing calculation to fully take into account this correction. Currently the mixing flag is only used for these three He-like lines, but in future it may be applied to other cases as well.

At the moment flags D (dielectronic recombination, cf. §2.4), P (photo-excitation, cf. §2.7) and C (charge-transfer recombination, cf. §2.8) are still put to zero.

The line parameter file is given in Appendix A (document SRON/SPEX/TRPB04a).

In the following paragraphs the seven processes contributing to the line formation in ion Z^{+z} (i.e. Z = atomic number, ionization stage IO = z+1) are described.

2.2 Excitation

For excitation the flag E = 1. The algorithm for excitation lines is based upon Mewe (1972): The excitation cross section Q_{ij} from level i to level j is written as (Mewe 1972, eq. 4):

$$Q_{ij} = 4\pi a_0^2 \frac{2\pi}{\sqrt{3}} \left(\frac{E_{\rm H}}{E_{ij}}\right)^2 f_{ij} \frac{g(U)}{U}, \qquad (1)$$

where $E_{\rm H}$ (= 13.6056981 keV) is the ionization energy of Hydrogen, a_0 is the Bohr radius, E_{ij} is the excitation energy, f_{ij} is the absorption oscillator strength of the transition, E is the initial energy of the impinging electron, $U = E/E_{ij}$ and $g(U)$ is the energy-dependent excitation Gaunt factor. Integration of (1) over a Maxwellian distribution leads to the total excitation rate S_{ij} (Mewe 1972,

eq. 6):

$$S_{ij} = \sqrt{\frac{8kT}{\pi m_e}} y^2 \int_1^\infty Q_{ij} e^{-yU} U \, \mathrm{d}U, \tag{2}$$

where $y = E_{ij}/kT$. By defining the Maxwellian-averaged Gaunt factor $\bar{g}(y)$ as (cf. Mewe 1972, eq. 8)

$$\bar{g}(y) = y e^y \int_1^\infty g(U) e^{-yU} \, \mathrm{d}U, \tag{3}$$

we can substitute (1) and (3) into (2) and obtain

$$S_{ij} = \frac{2^{9/2} \pi^{3/2} a_0^2 E_\mathrm{H}^2 f_{ij}}{3^{1/2} m_e^{1/2} (kT)^{1/2} E_{ij}} e^{-y} \bar{g}(y). \tag{4}$$

By taking energy E_{ij} and temperature T in keV and expressing S_{ij} in units of 10^{-20} m^3 s^{-1} we obtain from (4)

$$S_{ij} = 5.000965 \times 10^4 \frac{f_{ij}}{T^{1/2} E_{ij}} e^{-y} \bar{g}(y), \tag{5}$$

where now $y = E_{ij}/T$ with

$$E_{ij}\,[\mathrm{keV}] = a_\mathrm{EX} \frac{12.3984}{\lambda[\mathrm{Å}]}. \tag{5a}$$

Here $a_\mathrm{EX} = E_{ij}/E_\mathrm{line}$, and

$$E_\mathrm{line}[\mathrm{keV}] = \frac{12.3984}{\lambda[\mathrm{Å}]}, \tag{5b}$$

is the line photon energy. Note that the forefactor in eq. 5 is 1.7036 10^{-3} if we express T in K (1 K = 8.617385 10^{-8} keV), E_{ij} in eV and S_{ij} in cm^3 s^{-1}.

The line strength of a given transition from level j back to level k in ion Z^{+z} (not necessarily equal to the original level i) is given by

$$P_{jk}^\mathrm{exc} = S_{ij} BCC_\mathrm{ion}, \tag{6}$$

where P_{jk}^exc is in units of 10^{-20} m^3 s^{-1}, $B \equiv A_{jk} / \sum_{\ell \le j} A_{j\ell}$ is the branching ratio (column 10 in LINEPAR.ASC) of the transition (A's are radiative transition probabilities), and C is a cascade correction (column 11 in LINEPAR.ASC) for the population of level j by cascades from higher levels (this factor is in principle temperature-dependent, but the temperature dependence is neglected here). Finally, C_ion is the concentration of the radiating ion Z^{+z} relative to the Hydrogen concentration (thus C_ion is dimensionless!).

We introduce here a constant q_{jk} (units keV^{-1}) equal to

$$q_{jk} = \frac{f_{ij} BC}{E_{ij}} = \frac{f'_{jk}}{E_\mathrm{line}}, \tag{7}$$

where the corrected oscillator strength

$$f'_{jk} = \frac{f_{ij} BC}{a_\mathrm{EX}}, \tag{7a}$$

which was used in the old code in the expression for the line strength.

Using the constant q_{jk} (which can easily be derived from the parameters λ, f' and a_{EX} given in the database LINEPAR.ASC), the line strength is given by

$$P_{jk}^{\rm exc} = \alpha\ T^{-\frac{1}{2}} C_{\rm ion} e^{-y} \bar{g}(y), \tag{8}$$

where the parameter

$$\alpha = 5.000965 \times 10^4\ q_{jk}, \tag{8a}$$

is in keV^{-1} and $y = \beta/T$ with the excitation energy β (in keV):

$$\beta = a_{\rm EX} \frac{12.3984}{\lambda[\text{Å}]}, \tag{8b}$$

The excitation gaunt factor is calculated by putting (cf. Mewe and Gronenschild (1981) (hereafter MG81 or paper IV), eqs. 26 and 27):

$$g(U) = A + \frac{B}{U} + \frac{C}{U^2} + \frac{2D}{U^3} + E \ln U, \tag{9}$$

which leads after insertion into (3) to

$$\bar{g}(y) = A + (By - Cy^2 + Dy^3 + E) e^y E_1(y) + (C + D)y - Dy^2, \tag{10}$$

where

$$E_1(y) \equiv \int_1^\infty z^{-1} e^{-yz} dz, \tag{10a}$$

is the exponential integral. This is evaluated using Abramowitz and Stegun (1970) (eqs. 5.1.53 and 5.1.54) (for $y < 1$, the absolute accuracy is better than 2×10^{-7}; for $y > 1$, the relative accuracy is better than 5×10^{-5}). The mean Gaunt factor $\bar{g}(y)$ is evaluated using a subroutine in LINEM. The excitation parameters A, B, etc. are given in LINEPAR.ASC. Note that the original tables of Mewe and Gronenschild (1981) and Mewe *et al.* (1985) contain $2D$, whereas LINEPAR.ASC now contains D.

Finally we note that for the He-like forbidden line the ($n > 2$) cascade correction is currently done within the program (instead of being 'absorbed' into the coefficient f'_{jk}). It is given by eq. (28) of paper IV and eq. (37) of this document. The quantity r entering that equation is contrary to the old code not calculated using the approximation of eq. (29) of paper IV, but using the exact uncorrected excitation rates as calculated by the program using eq. 5.

2.3 Radiative recombination

For recombination the flag R = 1. The formula as used by Mewe *et al.* (1985) (hereafter MGO85 or paper V), (eq. A.9) for the rate coefficient (in cm^3 s^{-1}) of the contribution to the line strength from radiative recombination of ion $Z^{+(z+1)}$ of a spectral line in ion Z^{+z} is:

$$\alpha_{z+1}^{\rm RR} = 10^{-11}\ AREC\ (z+1)^{2\eta+1} T^{-\eta}, \tag{11}$$

where the electron temperature is in K. The constants $AREC$ and η (cf. Table I of paper V) are given in LINEPAR.ASC (note that $AREC$ includes the line branching ratio BR). In the current version we now use for the line strength

$$P^{\rm rec} = \alpha T^{-\eta} C_{\rm ion}, \tag{12}$$

where $P^{\rm rec}$ is in units of 10^{-20} m^3 s^{-1}, T in keV and $C_{\rm ion}$ is the concentration of the recombining ion $Z^{+(z+1)}$ relative to Hydrogen. The constant α is pre-calculated now as follows:

$$\alpha = 10^3\ AREC\ (z+1)^{2\eta+1}\ (8.617385\ 10^{-8})^{\eta}, \tag{13}$$

where we used the conversion ($\times\ 10^{14}$) from cm^3 s^{-1} to 10^{-20} m^3 s^{-1} and T is now in keV instead of K (1 K = 8.617385 10^{-8} keV).

Note: for all helium-like $n = 2$ He4 (w), He5 (x and y) and He6 (z) lines, this expression also includes the dielectronic recombination contribution! In a future version, this contribution ought to be separated.

2.4 Dielectronic recombination

In the process of dielectronic recombination, a free electron (labeled 1) collides with an ion; electron 1 is captured while exciting a bound electron (labeled 2). Dielectronic recombination occurs if electron 2 decays to a lower level by a radiative transition (contrary to the other possibility of auto-ionization). Such a radiative transition of electron 2 causes a dielectronic satellite line (treated in §2.4). After the emission of electron 2, electron 1 may decay leading to the line emission treated here.

In the original code Mewe and Gronenschild (1981) (paper IV) treated the contribution from dielectronic recombination captures into $n \geq 2$ states which lead to an additional population of the upper levels of the helium-like resonance (w), intercombination ($x+y$), and forbidden (z) lines and used for the line strength $P^{\rm dil}$ (in units 10^{-20} m^{-3} s^{-1}) a formula of the type:

$$P^{\rm dil} = [\alpha_1 e^{-\beta_1/kT} + \alpha_2 e^{-\beta_2/kT}] C_{\rm ion}, \tag{14}$$

where $C_{\rm ion}$ is the concentration of the recombining ion $Z^{+(z+1)}$ relative to Hydrogen, and α and β are constants which can be calculated from MG81 (eqs. (38), (42) and table XI). The second term in eq. (14) represents the cascade correction.

We remark that in the current version of the code no dielectronic recombination is taken explicitly into account, i.e. the flag D is always put to zero. Only in the case of the helium-like lines He4 (w) , He5 (x and y) and He6 (z) of all considered elements we implicitly include a contribution from dielectronic recombination in the radiative recombination and use eq. (12) (cf. also Mewe *et al.* (1985), §A1.4).

2.5 Dielectronic recombination satellites

Following Gabriel (1972) we write for the rate coefficient for the production by dielectronic recombination of ion $Z^{+(z+1)}$ of a satellite line in ion Z^{+z}:

$$\alpha^{\rm DR}_{z+1} = 4\pi^{3/2} a_0^3 \left(\frac{E_{\rm H}}{kT}\right)^{3/2} B_s e^{-E_s/kT} = 2.0706\ 10^{-16} T^{-3/2} B_s \exp(-E_s/kT), \tag{15}$$

where

$$B_s = \frac{g_s A_a A_r}{g_1 (A_a + \sum A_r)}. \qquad (15a)$$

Here the rate coefficient $\alpha^{\rm DR}_{z+1}$ is in units of cm^3 s^{-1}, the branching ratio parameter B_s in s^{-1}, and the electron temperature T in K; g_s and g_1 are the statistical weights of the satellite state in the recombined ion Z^{+z} and of the ground state in the recombining ion $Z^{+(z+1)}$, respectively; E_s is the energy difference between these two states (=kinetic energy of the plasma electron being captured by ion $Z^{+(z+1)}$). Further, A_a and A_r are transition probabilities (s^{-1}) by autoionization and radiation, and the summation is over all possible radiative transitions from the satellite level s. For a group of satellites with the same principal quantum number n for the spectator electron MG81 (eq. 40) approximate the satellite energy E_s as:

$$E_s[\mathrm{eV}] = 1.23984\ 10^4 \mathrm{a_{DR}}/\lambda[\mathrm{\AA}], \qquad (15b)$$

where λ is the wavelength of the satellite line and $a_{DR} = 0.7$, 0.86, 0.02, and 0.96 for $n = 2$, 3, 4, and > 4, respectively (cf. Appendix B, Table 1). The parameters n and $a_{\rm DR}$ are given in the datafile LINEPAR.ASC (columns 5 and 13).

In the current code we write (15) alternatively as:

$$\alpha^{\rm DR}_{z+1} = 5.238049 \times 10^{-13}\ T^{-3/2} B_s e^{-E_s/T}, \qquad (16)$$

where now the rate coefficient is in units of 10^{-20} m^3 s^{-1}, B_s in s^{-1} and T and E_s are in keV.

Mewe *et al.* (1985) have based their rate coefficients mainly on the data obtained for iron ($Z = 26$) and introduced for the branching ratio parameter B_s the following Z-scaling (their eq. (A.11)):

$$B_s(Z) = f(Z)\ B_s(26), \qquad (17)$$

with

$$f(Z) = \frac{10^{-6} b_5 (Z-1)^4}{1 + b_6 (Z-1)^4}. \qquad (17a)$$

By definition: $f(26) = 1$. Parameters b_5 and b_6 are given in Table 1 of Appendix B.

For the DR satellites MGO85 introduced in the old software a normalization factor $C_{\rm DR}$ (of the order unity) which turns out to be related to B_s (in units of s^{-1} and not in 10^{13} s^{-1} as was used by MG81 and MGO85!) by

$$C_{\rm DR} = 3.207\ 10^{-15} B_s(26) b_5. \qquad (18)$$

$C_{\rm DR}$ represents the satellite intensity of a given element (Z) scaled to the corresponding iron ($Z = 26$) case (cf. also Appendix B) (note that $C_{\rm DR}$ already includes the parameter b_5).

In the current version of the code the line strength $P^{\rm drs}$ (in units of 10^{-20} m^{3}s^{-1}) is given by

$$P^{\rm drs} = \frac{\alpha}{T^{3/2}} e^{-\beta/T} C_{\rm ion}, \qquad (19)$$

where $C_{\rm ion}$ is the concentration of the recombining ion $Z^{+(z+1)}$ relative to Hydrogen, and α (in units of 10^{-20} m^3 s^{-1} keV$^{3/2}$) and β (in keV) are constants which are pre-calculated from the data described above and below; T is in keV. Note that the satellite transition takes place in the recombined ion!

We distinguish in our code two types of dielectronic satellites:

Flag S = 1:

Dielectronic recombination (DR) satellites characterized by the parameter $C_{\rm DR}$ given in LINEPAR.ASC (column 21).

We note that in some cases the DR satellites have also a contribution from innershell excitation (i.e. flag E = 1).

From eqs. (16)–(19) we obtain for the constant α:

$$\alpha = 1.6333\ 10^{-4}\ C_{\rm DR} \frac{(Z-1)^4}{1+b_6(Z-1)^4}, \tag{20}$$

where $b_6 = 5\ 10^{-6}$, $3\ 10^{-5}$, and $5\ 10^{-5}$ for $n = 2$, 3, and $\geq$4, respectively (cf. Table 1 of Appendix B).

Comparing eqs. (15), (15b), and (19) we obtain:

$$\beta = a_{\rm DR} \frac{12.3984}{\lambda[\text{Å}]}. \tag{20a}$$

Appendix B (document SRON/SPEX/TRPB04b) contains a recently compiled list of more than 1000 dielectronic recombination satellite lines covering the wavelength region 1.53–41.57 Å. In this Appendix more details are given about the formulae used.

Flag S = 2:

'Unresolved' satellites are treated for the resonance transitions using MG81, eqs. (43-45). For the satellites other than case S=1 they have assumed that the satellites to a resonance line in ion Z^{+z} which are formed by DR of this ion and occur in ion $Z^{+(z-1)}$ are spectroscopically unresolved from the corresponding main resonance line and thus are lumped in with this line. Note, however, that their equation (43) contains a printing error and some unclearness: the constant should be 8.133×10^{-13} instead of 8.14×10^{-14}, their electron temperature $T_{\rm e}$ must be expressed in units of 10^6 K and the excitation energy χ_z^E in eV. Equation (43) of MG81 was adapted from the original semi-empirical Burgess (1965) formula with some corrections. We took the adapted Burgess formula, and wrote it in the following form, consistent with units and constants of eq. (19):

$$\alpha = 65.0615 A(x) B(z) f{\rm BR} C_{\rm DRS} \sqrt{\chi}, \tag{21}$$

where $\chi \equiv E_{ij}$ is the excitation energy in keV as given by eq. 5a (we note that here the factor $a_{\rm EX}$ is always unity because we consider only close satellites to resonance lines); α is in units of 10^{-20} m^{3}s^{-1}keV$^{3/2}$, f is the absorption oscillator strength (column 9 in LINEPAR.ASC), BR is the branching ratio (column 10 in LINEPAR.ASC) and $C_{\rm DRS} = 0.6$, a reduction factor that takes into account that not all levels are auto-ionizing. The quantities $A(x)$ and $B(z)$ are given by MG81 (eq. 44), i.e.

$$A(x) = \frac{1}{1+0.105x+0.015x^2}, \tag{21a}$$

$$B(z) = \frac{z^{1/2}(z+1)^2}{(z^2+13.4)^{1/2}}, \tag{21b}$$

where $x = \chi/E_{\rm H}(z+1)$ with $E_{\rm H} = 0.0136056981$ keV. Similarly, for β we have

$$\beta = C(z)\chi \tag{22}$$

with $C(z)$ given by

$$C(z) = \frac{1}{1 + 0.019\frac{z^3}{(1+z)^2}}. \tag{23}$$

Note that MG81 in their eq. (45) have taken a constant 0.019 instead of the Burgess value 0.015 to accomodate the results of Gabriel (1972) and Bhalla *et al.* (1975).

2.6 Innershell ionization

MG81 (eqs. 13 and 14) have considered electron impact ionization from the inner $1s^2$ shell of an ion $Z^{+(z-1)}$ which contributes to the production in an optically thin plasma to the formation of a certain line in the next higher ion Z^{+z} (e.g. the Kα and Kβ lines). In the case of innershell ionization of a Li-like ion this process gives a contribution to the the forbidden He-like (He z) line (and at very high density also to the intercombination (He x and y) lines. On the basis of the formula of Lotz (1968) with $\zeta = 2$ (total number of electrons in the $1s^2$ shell) and assuming the upper line level to be populated in proportion to its statistical weight g_j MG81 (eq. 13) obtain for the rate coefficient:

$$S_{\rm II} = 6.49 \times 10^{-4} C_{\rm II} T^{-1/2} \chi^{-1} E_1(\chi/kT) \ ({\rm cm}^3\ {\rm s}^{-1}), \tag{24}$$

where the fluorescence yield (photons per ionization) is given by

$$C_{\rm II} = \frac{g_j}{\sum g_j} \frac{A_r}{A_a + \sum A_r}. \tag{24a}$$

Here $\sum g_j$ is the total statistical weight of the configuration to which level j belongs and A_a, A_r are transition probabilities for decay by auto-ionization and radiation, where the summation is over all possible spontaneous radiative transitions from level j. The electron temperature T is here expressed in K and χ is the ionization energy of the $1s^2$ shell of the ion expressed in eV. $C_{\rm II}$ is given in LINEPAR.ASC.

For a group of (Kα) satellite lines MG81 approximate χ as:

$$\chi[{\rm eV}] = 1.2398 \times 10^4 a_{\rm II}/\lambda[{\rm Å}], \tag{24b}$$

where λ is a mean value for the wavelength and $a_{\rm II} \simeq 1.1...1.3$ for all considered ions (cf. Table II of MG81: $a_{\rm II} = 1.296$ for the Li I sequence, $= 1.242{+}0.009(Z{-}26)$ for Be–F seq., and $= 1.164{+}0.008(Z{-}26)$ for Ne and higher seq.). Note that the constant $a_{\rm II}$ for the He-sequence as used in paper IV (1.293) was corrected to a new value in paper V (1.33). For the Kβ lines we introduce a correction by multiplying $a_{\rm II}$ with $\lambda_{{\rm K}\beta}/\lambda_{{\rm K}\alpha} \simeq [1 + 0.0041Z]^{-1}$. Therefore we treat the Kα and the Kβ lines separately.

We use the flag I = 1 for the Kα lines and for the innershell ionization contribution to the He-like lines, whereas for the Kβ lines I = 2.

For the case of the contribution to the He-like forbidden (z) and intercombination (x, y) lines we write (from Mewe and Schrijver (1978), eqs. (31) and (32)):

$$C_{\rm II} = 0.75\left[\frac{a + bn_e}{3n_{ec} + 4n_e}\right], \tag{25}$$

where for z: $a = 3n_{ec}$, $b = 1$ and for x, y: $a = 0$, $b = 3$, with $n_{ec} = 6\ 10^{12}(Z-2)^{4.3}$ cm^{-3} (or $0.06(Z-2)^{4.3}$ in units of 10^{-20} m^{-3}) the critical electron density beyond which the $1s^2 2p$ levels in the Li-like ion get coupled to the ground state $1s^2 2s$ by electron collisions. For the three lines x, y, and z the coefficients 0.75 are given in LINEPAR.ASC in the column 'CII', but the density correction within square brackets is calculated later in the program.

The fluorescence line strength $P^{\rm flu}$ (in units of 10^{-20} m^3 s^{-1}) is given by

$$P^{\rm flu} = \alpha T^{-1/2} E_1(\beta/T) C_{\rm ion}, \tag{26}$$

where $E_1(y)$ is the exponential integral (see eq. 10a) and $C_{\rm ion}$ is the concentration of the ionizing ion $Z^{+(z-1)}$ relative to Hydrogen. The parameter α includes the fluorescence yield $C_{\rm II}$ which is given in the parameter file LINEPAR.ASC. We have with χ and T in keV for α (in units of 10^{-20} m^3 s^{-1} keV$^{1/2}$) and β (in keV):

$$\alpha = 1.9052 \times 10^4\ C_{\rm II}\ \chi^{-1}, \tag{26a}$$

and

$$\beta \equiv \chi = a_{\rm II}\frac{12.3984}{\lambda[\text{Å}]}. \tag{26b}$$

In Appendix C (document SRON/SPEX/TRPB04c) we give an extended list of Kα and Kβ lines compiled from a recent publication by Kaastra and Mewe (1993).

2.7 Photo-excitation

This process will be incorporated later when the calculations are applied to photo-ionized plasmas. Therefore the current flag P = 0. Here we write down the relevant formulae and often refer to Rybicki and Lightman (1979) (hereafter RL79).

We consider photon line excitation in an ion from level i towards level j due to an external radiation field and introduce the line absorption coefficient (per unit length and per unit frequency) at frequency ν (cf. RL79, eq. 1.74):

$$\alpha_\nu = \frac{h\nu}{c} n_i B_{ij}\, \phi(\nu), \tag{27}$$

where n_i is the number density of ions in state i, B_{ij} is the Einstein coefficient for absorption and $\phi(\nu)$ is the line profile function, which is sharply peaked at $\nu = \nu_0$ and which is conveniently taken to be normalized:

$$\int_0^\infty \phi(\nu) d\nu = 1. \tag{27a}$$

We have neglected here stimulated emission (cf. RL79, eq. 1.75) and we note that our formula differs from RL79 by a factor $4\pi/c$ because we use a different definition of B_{ij}. Then the number of photo-excitations $\mathcal{N}_{ij}$ per unit volume and per unit time in an ion embedded in a radiation field of energy

density u_ν (energy (volume)$^{-1}$ (frequency)$^{-1}$) - or alternatively, irradiated by a photon number flux $F_\nu (= \frac{cu_\nu}{h\nu})$ (photons per unit time, area and frequency) - can be written as

$$\mathcal{N}_{ij} = \int_0^\infty \alpha_\nu F_\nu d\nu = c \int_0^\infty \frac{\alpha_\nu u_\nu}{h\nu} d\nu = n_i \mathcal{B}_{ij}, \tag{28}$$

where

$$\mathcal{B}_{ij} = B_{ij} \int_0^\infty \phi(\nu) u_\nu d\nu \simeq B_{ij}\, u_{\nu_0}, \tag{28a}$$

is the rate (in units s^{-1}) for absorption (photo-excitation) $i \rightarrow j$. We assume here that $\phi(\nu)$ behaves like a δ-function so that the incident radiation flux changes only slowly over the width of the narrow line profile. We note that if we would replace in eq. 28a u_{ν_0} by the intensity J_{ν_0} $(= (c/4\pi)u_{\nu_0})$ we would obtain eq. 1.67 of RL79 which just gives the difference of the factor $4\pi/c$. Taking this into account we derive from RL79, eq. 10.29a:

$$B_{ij} = \frac{\alpha c f_{ij}}{2 m_e \nu_0}, \tag{29}$$

where $\alpha = 0.00729735308$ is the fine-structure constant and f_{ij} is the absorption oscillator strength. Substituting (29) into (28) we find

$$\mathcal{N}_{ij} = \alpha (h/2m_e) n_i F_{\nu_0}. \tag{35}$$

Expressing the photo-excitation rate $\mathcal{N}_{ij}$ in m^{-3} s^{-1}, ion density n_i in 10^{20} m^{-3}, photon flux F_E (at photon energy $E = h\nu_0$) in 10^{28} phot m^{-2} s^{-1} keV^{-1} and using $h/2m_e = 3.63694807\ 10^{-4}$ m^2 s^{-1} and $10^3 e/h = 2.41798836\ 10^{17}$ A J^{-1} (conversion from Hz to keV), we obtain

$$\mathcal{N}_{ij} = 1.097611\ 10^{25}\ n_i f_{ij} F_E. \tag{30a}$$

By applying the relations between the Einstein coefficients B_{ij} and A_{ji} (RL79, eq. 1.72b, but again with additional factor $4\pi/c$) we rewrite eq. 28a:

$$\mathcal{B}_{ij} = \frac{g_j}{g_i} A_{ji} \frac{c^3}{8\pi h \nu_0^3} u_{\nu_0}, \tag{31}$$

where A_{ji} is the spontaneous radiative transition probability (s^{-1}) and g_j and g_i are the statistical weights of levels j and i. As an example we treat the case of a diluted blackbody (BB) radiation field with radiation temperature T_r, because we apply this to the mixing of helium-like lines (cf. §4.):

$$u_\nu = \frac{8\pi h \nu^3}{c^3} W [e^{h\nu/kT_r} - 1]^{-1}. \tag{32}$$

Then we obtain for the absorption rate

$$\mathcal{B}_{ij} = \frac{W A_{ji} (g_j/g_i)}{e^{h\nu/kT_r} - 1}, \tag{33}$$

where W is the dilution factor. For example, $W = 1$ for pure BB radiation ('hollow cavity'), $W = \frac{1}{2}$ close to the surface of a star with BB-type radiation from the photosphere with characteristic radiation

temperature T_r, or at a distance d from the center of the star (with radius R_*) (cf. eq. 51 of Mewe and Schrijver (1978), hereafter MS78):

$$W = \frac{1}{2}[1 - \{1 - (R_*/d)^2\}^{1/2}]. \tag{34}$$

2.8 Charge-transfer (recombination) processes

This process will be incorporated later when we consider the case of photo-ionized plasmas. Therefore the current flag C=0. Here we only briefly deal with these processes.

Charge-transfer reactions can be very important in very cool photo-ionized plasmas (i.e. electron temperature $T \lesssim 10^4$ to 10^5 K). Charge-transfer ionization and recombination can play an important role in determining the ionization structure in such plasmas and especially charge-transfer recombination may be significant in the population of the upper line levels via cascades from higher states.

In plasmas with cosmical abundances (i.e. hydrogen and helium dominant) usually only recombination reactions like

$$\mathrm{A}^{+z} + \mathrm{B}^0 \rightarrow \mathrm{A}^{+(z-1)} + \mathrm{B}^+$$

exist, B being either H or He. They proceed via electron transfer to an excited level of $\mathrm{A}^{+(z-1)}$.

3 Electron density correction for single lines

If the uncorrected line strength of a particular line is S_0, the density-corrected value is given by

$$S = S_0(1 + D_\mathrm{n}), \tag{35}$$

where D_n is the electron density-sensitive correction term.

In the input line data file LINEPAR.ASC we use flag N to indicate the density correction. If N > 0 then with N = i we indicate equation (i) in the computer program corresponding here in the following description to equation (35.i).

3.1 Helium-like lines

The density effect of the intercombination and forbidden lines of the He I iso-electronic sequence is taken into account by the calculation of the detailed coupling of these lines (cf. §4). However, approximation formulae have been derived for the lines from C V – S XV (wavelength region 5–42 Å): Eq. (A.14) in paper V for the forbidden lines and Eq. (A.1) in Mewe *et al.* 1991 for both intercombination and forbidden lines. The latter reads:

$$D_\mathrm{n} = \frac{1 + \alpha n_e}{1 + \beta n_e} - 1, \tag{35.1}$$

where α and β are parameters given in the parameter file and n_e is the electron density in units of 10^{20} m^{-3} ($= 10^{14}$ cm^{-3}). In order to avoid too large parameters we use in the case of the He-like lines from C, N, and O a slightly modified formula (in order to avoid too large parameters in LINEPAR.ASC):

$$D_{\rm n} = \frac{1 + 10^3 \alpha n_e}{1 + 10^3 \beta n_e} - 1. \tag{35.2}$$

3.2 Iron and nickel lines

For a number of iron satellite lines around 1.9 Å from the C, N, and O I iso-electronic sequences (Fe XXI–XIX) we use also Eq. (35.1).

MGO85 (paper V) use 3 different formulae to model the density correction for spectral lines of iron and nickel from the Be, B, C, N, O, and F I iso-electronic sequences (Fe XXIII–XVIII and Ni XXIV–XXI, covering the wavelength regions 7–13 Å and 90–140 Å) (cf. their eqs. A.12–13 and cf. also Mewe *et al.* (1991), eqs. A.2–4). We give here the same formulae, but with a slightly different notation.

$$D_{\rm n} = \alpha(1 - e^{-\beta n_e^{\gamma}}), \tag{35.3}$$

corresponding to eq. (A.12a) or (A.3), which is used for the Be, C, N, O, and F I sequences. Because we use different units for n_e (in the old form 10^{12} cm^{-3}) we have the conversion $\beta = 10^{2\gamma}\ \beta'$ ($'$ indicates the old parameters), whereas α and γ are the same as in the old formulae. In one case (the iron C7f line) where we want to avoid a too large value of the parameter β we use the slightly modified formula:

$$D_{\rm n} = \alpha(1 - e^{-10^2 \beta n_e^{\gamma}}). \tag{35.4}$$

For the C I sequence we use in some cases (cf. eq. A.12b or A.4):

$$D_{\rm n} = \frac{\alpha}{1 + 0.1107 n_e^{-3/4}}, \tag{35.5}$$

where $\alpha = \delta'$ (= the parameter in the old formula).

For the B I sequence we use (cf. eq. A.13 or A.2):

$$D_{\rm n} = \frac{\alpha}{n_e^{0.03} + T^{-0.3} n_e^{-1}}, \tag{35.6}$$

where again T is in keV (instead of K) and $\alpha = 0.8714\alpha'$.

4 Mixing and coupling of lines

This discussion is relevant to the intercombination line (i) and the 'forbidden' (not strictly!) line (f) (or z) of the He I iso-electronic sequence. In the current version of the code the intercombination line is now splitted in its two components x and y for all considered elements but here we deal first with the unsplitted case, i.e. i denotes the total ($x + y$) intercombination line. Notations x, y, z are from Gabriel (1972).

4.1 Intercombination lines lumped together

For these lines, coupling between the lines was calculated using eqs. (16)–(20) of paper IV. Those equations were applied to innershell ionization, but were also applied to other possible emission processes for these lines. We repeat here the equations for the case of excitation. The effective rate coefficients read for the forbidden $2^3S_1 \rightarrow 1^1S_0$ line (f) and for the intercombination line $2^3P \rightarrow 1^1S_0$ (i):

$$S^{eff}_{f,\mathrm{EX}} = [S'_{f,\mathrm{EX}} + (1 - BR_i)S'_{i,\mathrm{EX}}]BR_f, \tag{36a}$$

$$S^{eff}_{i,\mathrm{EX}} = S'_{i,\mathrm{EX}}BR_i + [S'_{f,\mathrm{EX}} + (1 - BR_i)S'_{i,\mathrm{EX}}](1 - BR_f), \tag{36b}$$

where $S'_{f,\mathrm{EX}}$ and $S'_{i,\mathrm{EX}}$ are the excitation rate coefficients without coupling effects, but including ($n > 2$) cascade corrections (denoted by $'$), i.e. $S' = SC$, where S is described by eq. (5) and C is the cascade correction given by (cf. eq. 28 of paper IV) for the forbidden line:

$$C_f = 1 + 0.4\ r\ \exp(-0.21y), \tag{37}$$

where $y = E_{\mathrm{EX}}/kT$ (E_{EX} the excitation energy of the forbidden line) and $r = S_{i,\mathrm{EX}}/S_{f,\mathrm{EX}}$ the ratio of the excitation rates without cascades as calculated by eq. 5. For the intercombination line we have $C_i = 1.065$ (also given in LINEPAR.ASC).

Further,

$$BR_i = \frac{A_{ig}}{A_{ig} + A_{if}}, \tag{38}$$

is the branching ratio of the intercombination line to the ground state (g) (A_{ig} denotes the transition probability for the spontaneous radiative transition $i \rightarrow g$ ($2^3P_k \rightarrow 1^1S_0$), etc. ($A$'s were taken from MS78). BR_i is given in Table III of MG81 (and approximated by MGO85 for $Z \gtrsim 7$ by $BR_i \simeq 0.09Z^{0.57}$).

The branching ratio BR_f of the forbidden line to the ground state is more complicated. It is unity at low electron density (n_e) (in LINEPAR.ASC we give $BR_f = 1$), but at high densities or in a strong radiation field the upper level of the forbidden line will be coupled to the next higher levels (= the upper levels of the intercombination lines) which causes a decrease of the branching ratio. This case is treated in detail by MS78, but here we give their results approximated by MG81 (eqs. 18–20):

$$BR_f = \frac{A_{fg}}{A_{fg} + (n_e S_{fi} + \mathcal{B}_{fi})BR_i} = \frac{1}{1 + (\beta_c n_e + \beta_r)BR_i}, \tag{39}$$

where $\beta_c = S_{fi}/A_{fg}$ and $\beta_r = \mathcal{B}_{fi}/A_{fg}$; S_{fi} is the excitation rate coeffcient for collisional excitation from 2^3S to 2^3P, A_{fg} the transition probability for transition $2^3S_1 \rightarrow 1^1S_0$, and $\mathcal{B}_{fi}$ the absorption rate coefficient (s^{-1}) in an external radiation field (cf. eq. 28a) which causes a transition from 2^3S to 2^3P. We use the approximation from MG81:

$$\beta_c \simeq 330Z^{-14.57}\left(\frac{T}{10^5Z^2}\right)^{-0.73Z^{-0.415}} \quad (\mathrm{cm}^3), \tag{40a}$$

where Z is the atomic number and T in K. The inverse of $\beta_c BR_i$ is the critical electron density above which collisional excitation from 2^3S to 2^3P begins to dominate over the 'forbidden' radiative decay from the metastable level 2^3S to the ground state 1^1S. We note that in the current code β_c is expressed in units of 10^{-20} m^3 so that then the forefactor in eq. 40a reads: $330 \times 10^{14} \times (8.617385\ 10^{-8})^{0.73Z^{-0.415}}$.

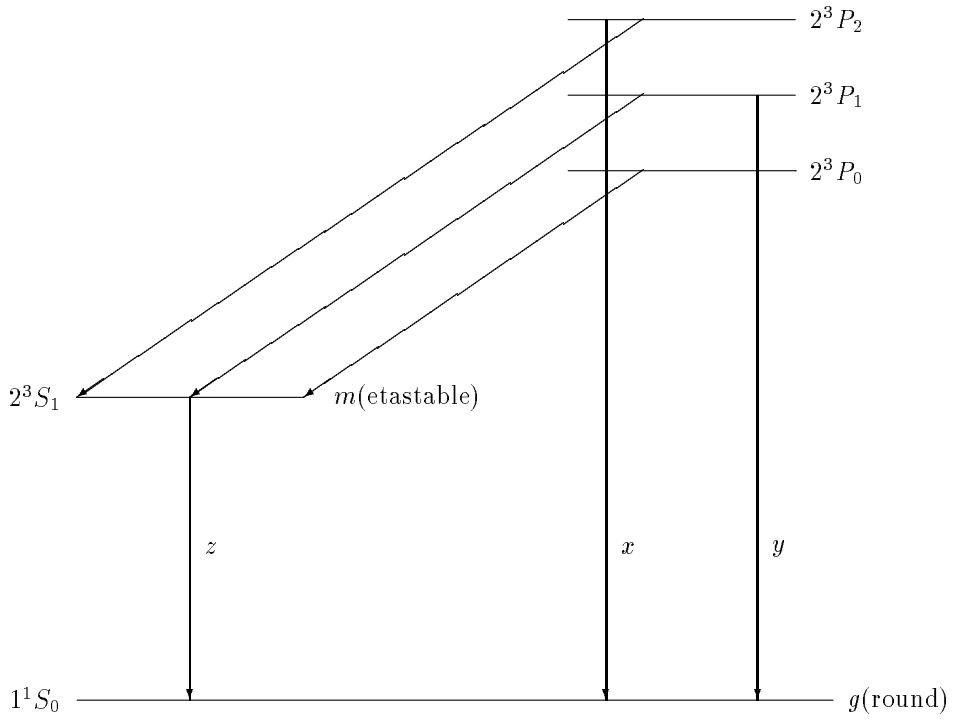

Figure 1: Energy level and transition scheme of He-like $n = 2$ triplet lines: the intercombination lines x ($2 \rightarrow g$, or shortly $2g$), y ($1g$) (the transition $0g$ is strictly forbidden), and the 'forbidden' line z (mg). The arrows indicate the spontaneous radiative transitions. In the calculations the coupling between the levels 2^3S_1 and 2^3P_j ($j = 2, 1, 0$) is assumed to occur from $2^3P_{2,1,0}$ to 2^3S by spontaneous radiative transitions (rates $A_{j\,m}$) (neglecting collisional de-excitation and stimulated emission) and from 2^3S to $2^3P_{2,1,0}$ by electron collisions (rates $n_e S_{mj}$) and photo-excitation (rates $\mathcal{B}_{mj}$).

For the radiation field MS78 considered diluted blackbody-type radiation from the photosphere of a star, characterized by an effective radiation temperature T_r and a dilution factor W ($\simeq 1/2$ close to the star, cf. eq. 51, MS78 and eq. 33 of this document). Then MG81 write:

$$\beta_r = \frac{\beta_1 W}{e^{\beta_2/T_r} - 1}, \tag{40b}$$

where the parameters β_1 and β_2 are given in Table IV of MG81 (note that β_1 was wrongly calculated).

For the case of zero radiation field Mewe *et al.* (1991) have derived the approximate formula (35.1) to describe the density behaviour of f (or z) and i (or $x + y$).

4.2 Splitting of intercombination lines

Now we carry out in the above formulae the proper splitting of the intercombination line i into the two components x and y ($2^3P_j \rightarrow 1^1S_0$ with $j = 2$ for x and $j = 1$ for y; the lowest level 2^3P_0 does not couple radiatively to the ground state 1^1S_0 but it does to the metastable 2^3S_1 state) (cf. Fig. 1.). In LINEPAR.ASC the branching ratios (BR_x and BR_y) are given separately for the two components x and y. The mixing flag M is put 1,2,3 for x, y, z, respectively.

We follow the detailed solution given by MS78 and introduce the following notations (cf. also Fig. 1.):

Upper level of the forbidden line (z): $2^3S_1 \equiv m$; upper level of an intercombination line ($j = 2$ for x, 1 for y): $2^3P_j \equiv j$; the ground level: $1^1S_0 \equiv g$. E.g., the transition $2^3P_j \rightarrow 2^3S_1$ is shortly denoted by jm, etc.

The branching ratio for level k to level ℓ (i.e. the fraction which goes from k to ℓ) with respect to other levels is denoted by $BR_{k\ell}$, etc.

From MS78 (eqs. 20–25, 38–41) we derive for the effective rate coefficient of the forbidden line $m \rightarrow g$ an expression analogous to eqs. 36a and 37:

$$S_{gm}^{eff} = BR_{mg} \left[S'_{gm} + \sum_{j=0}^{2} S'_{gj} BR_{jm} \right], \tag{41}$$

where the first term within the brackets represents the contribution from cascades from higher ($n > 2$) levels, whereas the second term gives the contribution from the 2^3P_j levels, weighted with the branching ratios BR_{jm} given by:

$$BR_{jm} = 1 - BR_{jg}, \tag{42}$$

where

$$BR_{jg} = \frac{A_{jg}}{A_{jg} + A_{jm} + n_e S_{jm} + B_{jm}} \simeq \frac{A_{jg}}{A_{jg} + A_{jm}}. \tag{42a}$$

Here we have neglected collisional and stimulated radiative de-excitation of the 2^3P levels. A_{jg} denotes the transition probability for transition $j \rightarrow g$, etc. The BR's were calculated using transition probabilities from Lin *et al.* (1977).

The branching ratios $BR_{2g} \equiv BR_x$ and $BR_{1g} \equiv BR_y$ are taken from LINEPAR.ASC, while $BR_{0g} \equiv 0$. In the case of the forbidden line in LINEPAR.ASC a formal value of 1 is given which is not used: the branching ratio $BR_{mg} \equiv BR_z$ is given by eq. 45 and calculated in the program.

In eq. 41 a $'$ denotes the inclusion of $n > 2$ cascades into the collisional rate coefficient, i.e.

$$S'_{gm} = C_{gm} S_{gm}, \quad S'_{gj} = C_{gj} S_{gj}, \tag{43}$$

where S denotes the excitation coefficient without cascades (and branching ratio). For the population of the 2^3P_j levels (intercombination lines) we approximate $C_{gj} = 1.065$ ($j = 2, 1, 0$) (in LINEPAR.ASC we give these cascade factors for x and y, i.e. $C_{g2} \equiv C_x$ and $C_{g1} \equiv C_y$ are both 1.065). For the

forbidden line we give in LINEPAR.ASC $C_{gm} \equiv C_z$ only formally the value 1, but in the program we calculate the full cascade contribution $C_{gm} \equiv S'_{gm}/S_{gm}$ from $n > 2$ levels via eq. 44a:

$$S'_{gm} = S_{gm} + 0.4 S_{g\Sigma} \exp(-0.21y), \tag{44a}$$

where $S_{g\Sigma} \equiv \Sigma S_{gj}$ is the total rate coefficient without cascades and branching ratio for collisional excitation from the ground state to all levels $2^3P_{2,1,0}$. Assuming that the excitation rates into the individual sublevels are divided according to the statistical weights g_j of the 2^3P_j levels ($g_j = 5, 3, 1$ for $j = 2, 1, 0$, respectively), we write:

$$S_{gj} = \frac{g_j}{\Sigma g_j} S_{g\Sigma} = \frac{g_j}{9} S_{g\Sigma}, \tag{44b}$$

Then we can obtain the total rate $S_{g\Sigma}$ from: $S_{g\Sigma} = \frac{9}{8}(S_x + S_y)$, and the rate to level 0 (= upper level of the "forbidden" intercombination line to the ground) S_{g0} from: $S_{g0} = \frac{1}{3} S_y$, where $S_x \equiv S_{g2}$ and $S_y \equiv S_{g1}$ are the excitation rates for the lines x and y without cascades and branching ratios as calculated in the program using eq. 5.

Finally, for the forbidden line we calculate the branching ratio $B_{mg} \equiv BR_z$ from:

$$BR_{mg} = \frac{A_{mg}}{A_{mg} + \sum_{j=1}^{2} (n_e S_{mj} + B_{mj})\, BR_{jg}} = \frac{1}{1 + \sum_{j=1}^{2} (\beta_{cj}\, n_e + \beta_{rj})\, BR_{jg}}, \tag{45}$$

where

$$\beta_{cj} = \frac{S_{mj}}{A_{mg}}, \tag{46}$$

and S_{mj} is the rate coefficient for collisional excitation $2^3S_1 \rightarrow 2^3P_j$. We could use the approximation $\beta_{cj} = \frac{g_j}{9}\beta_c$, where β_c is the total rate coefficient in the approximation given by eq. 40a. However we will use the formulae given by MS78 (see below). For the photo-excitation we write (cf. eqs. 33 and 40b):

$$\beta_{rj} = \frac{\mathcal{B}_{mj}}{A_{mg}} = \frac{\beta_{1j} W}{e^{\beta_2/T_r} - 1}. \tag{47}$$

The latter coefficients read (from eq. 33):

$$\beta_{1j} = \frac{A_{j\,m}(g_j/g_m)}{A_{mg}}, \quad \beta_{2j} = \frac{h\nu_{j\,m}}{k} = \frac{1.43877\ 10^8}{\lambda_{j\,m}}, \tag{48}$$

where the statistical weight of the 2^3S_1 level $g_m = 3$, the transition wavelengths $\lambda_{j\,m}$ in Å, and the radiation temperature T_r in K. We have calculated the β's using the A's from Lin *et al.* (1977) (A_{mg} from MS78) and wavelengths from Vainshtein and Safronova (1985). We must multiply β_{2j} with a factor $8.617385\ 10^{-8}$ if we express T in keV. In the program the β's of eq. 48 are stored in arrays with notation β_{11} = BETA1X, β_{21} = BETA2X, etc. Further β_{c1} = BETACX, etc.

Finally, for the electron collisional coefficients we derive from MS78 (eq. 42):

$$\beta_{cj}(T) \equiv \beta_{cej}(T) = C(Z-1)^{-2} T^{-1/2} \left[a^*_{mj} + b^*_{mj}\, e^{y_{ej}} E_1(y_{ej})\right] e^{-y_{ej}}, \tag{49}$$

with

$$y_{ej} = h\nu_{j\,m}/kT = \beta_{2j}/T, \tag{49a}$$

where the electron temperature T is in K and β_{2j} is given by eq. 48. In eq. 49 β_{cj} is in 10^{-20} m^3 and T now in keV. For the forefactor we have: $C = 10^{-4} \times 10^{14} \times (8.617385\ 10^{-8}) \times 10^{-6} = 2.9355$. Finally, $a^*_{mj} = 10^6 a_{mj}/A_{mg}$ and $b^*_{mj} = 10^6 b_{mj}/A_{mg}$, where the coefficients a_{mj} and b_{mj} and the transition probability A_{mg} are taken from MS78. In the program the coefficients a^* and b^* are stored in arrays and are called aMX,aMY,aM0 and bMX,bMY,bM0 for $j = 2, 1, 0$.

We note that the expression in square brackets in eq. 49 is calculated according to eq. 10 with $A = a^*_{mj}, B = C = D = 0, E = b^*_{mj}$ using subroutine GLINE.

The calculation of the intercombination line intensities is more complicated but proceeds straightforwardly from eqs. 20, 27–30 of MS78. We derive for the effective collisional rate coefficient of the intercombination line $j \rightarrow g$ ($j = 2, 1$ for x, y, respectively):

$$S^{eff}_{gj} = BR^*_{jg} \left[S'_{gj} + S'_{gm} BR_{mj} \right], \tag{50}$$

where the branching ratios for $j = 2, 1, 0$:

$$BR_{mj} = \frac{n_e S_{mj} + B_{mj}}{A_{mg} + \sum_{j=0}^{2} (n_e S_{mj} + B_{mj})} = \frac{\beta_{cj}\, n_e + \beta_{rj}}{1 + \sum_{j=0}^{2} (\beta_{cj}\, n_e + \beta_{rj})}, \tag{50a}$$

and again neglecting collisional and stimulated radiative de-excitation of levels j:

$$BR^*_{jg} = \frac{A_{jg}}{A_{jg} + A_{jm} BR^*_{mg}}, \tag{50b}$$

where

$$BR^*_{mg} = \frac{A_{mg}}{A_{mg} + \sum_{j=0}^{2} (n_e S_{mj} + B_{mj})} = \frac{1}{1 + \sum_{j=0}^{2} (\beta_{cj}\, n_e + \beta_{rj})} = 1 - \sum_{j=0}^{2} BR_{mj}. \tag{50c}$$

In the program: BR^*_{2g} = BRSTARXG, BR^*_{mg} = BRSTARMG, A_{2g} = AXG, A_{2m} = AXM (A's stored in arrays), BR_{m2} = BRMX, etc.

We introduce an additional correction on the rate coeffcients S_{mj} for electron collisional excitation $m \rightarrow j$ by taking into account the contribution from collisions with protons (p) and α-particles using eqs. 44–46 and Table 5 of MS78. We write for the total collisional coefficient:

$$\beta_{cj}(T, T_p, T_\alpha) = \beta_{cej}(T) + \beta_{cpj}(T_p) + \beta_{c\alpha j}(T_\alpha), \tag{51}$$

where

$$\beta_{cpj}(T_p) = \beta_{cj}(T = T_p)(N_{\rm H^+}/n_e) A_p Z \exp(-B_p Z/T_p), \tag{51a}$$

$$\beta_{c\alpha j}(T_\alpha) = \beta_{cj}(T = T_\alpha)(N_{\rm He^{++}}/n_e) A_\alpha \exp(-B_\alpha/T_\alpha), \tag{51b}$$

$$A_\alpha = 0.152(Z-1)^{1.056}, \quad B_\alpha = 1.29\ 10^6 (Z-1)^{1.073}. \tag{51c}$$

Here T_p and T_α are the kinetic temperatures (in K) of protons and α-particles. In eq. 51a,b $\beta_{cj}(T = T_x)$ is given by eq. 49 with the electron temperature T replaced by the particle temperature T_x ($x = p$ or α for protons or α-particles). For hot plasmas with cosmical abundances we can approximate:

$$\frac{N^+_{\rm H}}{n_e} \simeq \frac{1}{1 + 2A_{\rm He}}, \quad \frac{N^{++}_{\rm He}}{n_e} \simeq \frac{A_{\rm He}}{1 + 2A_{\rm He}}, \tag{52}$$

where $A_{\rm He}$ is the abundance of helium relative to hydrogen (e.g. $A_{\rm He} \simeq 0.1$). However, the proton and α-particle densities are calculated from the program.

We can apply eqs. 41 and 50 also to other processes than excitation, for example innershell ionization (II) if we make the following substitutions:

$$S'_{gm} \Longrightarrow \frac{N_{\rm Li}}{N_{\rm He}} S^{\rm II}_{g'm} = \frac{N_{\rm Li}}{N_{\rm He}} S^{\rm II}_{2^3S},$$

where $S^{\rm II}_{2^3S}$ is given by eq. 25, and $N_{\rm Li}$ and $N_{\rm He}$ are the concentrations of ions of the considered element in the Li-like and He-like ionization stage; g' is the ground state of the Li-like ion stage. The same for 2^3P excitation if we replace m by Σ.

For radiative plus dielectronic recombination (RR+DR):

$$S'_{gk} \Longrightarrow \frac{N_{\rm H}}{N_{\rm He}} \alpha^{\rm RR+DR}_{ck},$$

where c denotes the continuum above the He-like ion, and $N_{\rm H}$ is the concentration of H-like ions. We note that at the moment we incorporate recombination with eq. 13 and do not use the coupling scheme.

Note that in the current implementation, lines which are intermixing must be listed directly after each other, i.e. the line parameter file PARLIN cannot contain other independent lines listed in between intermixed lines. However, this is not the case for the original input data file LINEPAR.ASC because at the conversion to PARLIN the mixing lines from LINEPAR.ASC are selected in such a way that they are listed after each other in PARLIN.

5 Parameters

For line process 1 (excitation):

1 – α in keV^{-1} (cf. eq. 8a)

2 – β in keV (cf. eq. 8b)

3–7 – the excitation Gaunt factor parameters A, B, C, D and E; note that the original tables of Mewe and Gronenschild (1981) and Mewe *et al.* (1985) contain $2D$; the input file LINEPAR.ASC now contains D.

For line process 2 (radiative recombination):

1 – α (eq. 13)

2 – η (eq. 12)

For line process 3 (dielectronic recombination):

1 – α_1 (eq. 14)

2 – β_1 (eq. 14)

3 – α_2 (eq. 14)

4 – β_2 (eq. 14)

For line process 4 (dielectronic satellites):

1 – α (eq. 20)

2 – β (eq. 20a)

For line process 5 (innershell ionization):

1 – α (eq. 26a)

2 – β (eq. 26b)

For the density correction of single lines:

1–3 α, β, γ (eqs. 35)

For the mixing of coupled lines (He-like forbidden and intercombination lines):

1 – BR's (eqs. 42a, 45, 49a–c)

2– β_{cj1} in units of 10^{-20} m^3, if β_{cj} (cf. eqs. 39 and 46) is written as $\beta_{cj} = \beta_{cj1} T^{-\beta_{cj2}}$ with T the electron temperature in keV.

3 – β_{cj2} as above defined

4– β_{1j} (eq. 48)

5– β_{2j} in keV (eq. 48)

6– this parameter is 3 times the critical density n_{ec} (eq. 25), needed for innershell ionization of the He-like forbidden and intercombination lines. Units: as usual in 10^{20} m^{-3}.

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