

JPL PUBLICATION 77-11

(NASA-CF-152681) PROCESSED COMPUTER MODEL  
FOR ELECTRIC DISCHARGE PLASMA VAPOR DEPOSITS

A77-22461

CSCI 20E

Unclas

63/36

25145

National Aeronautics and  
Space Administration

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JPL PUBLICATION 77-11

# Proposed Computer Model for Electric Discharge Atomic Vapor Lasers

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March 15, 1977

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Prepared Under Contract No NAS 7-100  
National Aeronautics and Space Administration

PREFACE

The work described in this report was performed by the Control and Energy Conversion Division of the Jet Propulsion Laboratory.

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ABSTRACT

A detailed computer model for the rate kinetics of an atomic vapor laser excited by electrical discharge is proposed. The model equations are defined and the computer program structure is discussed.

PROPOSED COMPUTER MODEL FOR ELECTRIC DISCHARGE  
ATOMIC VAPOR LASERS

Introduction

It is the goal of the present program of computer modeling to numerically simulate the gross features of atomic vapor lasers excited by electrical discharge. Due to the inherent complexity of interactions in such a laser, the extent of attainment of this goal is uncertain. Nevertheless, much qualitative information on some of the processes taking place can be expected, leading to a better understanding of the physics of this laser type.

Limitations on computation time and computer program storage make inevitable considerable simplification of real processes or characteristics of the laser. As a first step, the proposed model focuses on rate processes, i.e., the change of electronic excited state populations through inelastic collisions and radiative interaction. Only temporal variations are included; the system is taken spatially homogeneous. In any particular atom or ion, levels of similar configuration (e.g. terms) are handled as a unit with populations assumed proportional to degeneracies. The set of level units of the atom or ion is split into three distinct groups: an upper subset in equilibrium with the free continuum states, a middle subset assumed quasistationary and a lower subset requiring numerical integration of rate equations to determine populations. The continuum plus the upper subset are treated together and will be called the "extended continuum" [1]. The relaxation times between states in the extended continuum and also in the quasistationary group are short relative to any other physical time of interest in the system. Populations in intermediate levels are small compared to the lower levels or the extended continuum. The occupation probability (based on equilibrium) is high for the low levels due to the Boltzmann factor and high for free or near free states due to large degeneracies. The short relaxation times and large possible population fluxes lead to equilibrium of extended continuum states among themselves. Fluxes in the quasistationary group are relatively small and the net rates into and out of a particular level are nearly the same;

populations change in a slow adiabatic manner so that they may be approximated by algebraically solving the rate equations assuming null rates [2]. It is assumed in the model that the degree of ionization of the laser gas is always sufficient (greater than  $10^{-4}$ ) to neglect the effects of atom-atom collisions on rates [1]; thus excited state equilibrium is characterized by the electron temperature without regard to heavy particle temperatures. This amount of ionization also assures a Maxwellian electron velocity distribution [2]. Neglect of atom-atom inelastic collisions in the rate equations does not mean that they are necessarily inconsequential in sublevel relaxation or relaxation between close levels in a unit. An equilibrium extended continuum also requires a sufficiently small charged particle mean free path.

### Rate Equations

Let the population of level unit  $n$ , specie  $s$  with parent ion core charge  $ze$  be  $N_n^{s,z}$ . The extended continuum is denoted by  $n^*$ ; the corresponding reference number density is  $N_{n^*}^{s,z} \equiv N_1^{s,z+1}$ . Note that the actual density of the extended continuum is

$$(1 + \epsilon z^{3/2}) N_1^{s,z+1}$$

where

$$\epsilon = N_e (\pi e^2 \ell_D / kT_e)^{3/2} / 3 \ll 1 \quad [1].$$

This holds for an extended continuum lower principal quantum number of about 5 to 7 and is based on the Debye lowering of ionization potentials [3]. Here  $N_e$  is the electron density and  $\ell_D$  is the Debye length. A Saha factor is defined as

$$\beta_n^{s,z}(T_e) = \frac{g_n^{s,z}}{2 g_1^{s,z+1}} \left( \frac{h^2}{2\pi m_e kT_e} \right)^{3/2} \exp(I_n^{s,z}/kT_e)$$

where the  $g$ 's are degeneracies,  $h$  the Planck constant,  $m_e$  the electron mass and  $I_n^{s,z}$  is the ionization potential of level  $n$ . At equilibrium,  $N_n^{s,z} = \beta_n^{s,z} N_e N_1^{s,z+1}$



with  $\beta_{n^*}^{S,Z} N_e \equiv 1$ . For hydrogenic levels, the preceding degeneracy factor equals the square of the principal quantum number. If the ionization rate coefficient from  $n$  is  $K_{n\infty}^{S,Z}(T_e)$ , the total excitation rate coefficient into the extended continuum is

$$K_{nn^*}^{S,Z} = K_{n\infty}^{S,Z} + \sum_{m>n^*} K_{nm}^{S,Z} .$$

Excitation coefficients  $K_{nm}$  are discussed in Appendix D. The maximum principal quantum number is  $(z\ell_D/2a_0)^{1/2}$ . At equilibrium,  $N_m K_{mn} = N_n K_{nm}$ , giving deexcitation coefficients. The net radiative emission rate  $m \rightarrow n$  is  $A_{mn} E_{mn}$  where  $A$  is the Einstein spontaneous emission coefficient and  $E$  is the escape factor (Appendix B). If a particular transition is coupled into the laser cavity,  $E$  is replaced by a factor dependent on the laser intensity (Appendix C). In the following,  $E$  will denote a generalized emission factor. The emission rate depends on the transition line profile unless the transition is optically thin; line profiles and broadening for the model are the topics of Appendix A.

A normalized population  $\bar{N}_n^{S,Z}$  is defined by  $N_n^{S,Z} \equiv N_e \beta_n^{S,Z} \bar{N}_n^{S,Z}$  so that at equilibrium  $\bar{N}_n^{S,Z} = N_1^{S,Z+1}$  (all  $n$ ). Also,  $R_n^{S,Z} = (d/dt) \bar{N}_n^{S,Z}$  and  $R_e = (d/dt) \ln N_e$  are net rate functions.

For  $n < n^*$ , the basic rate equations for an atom or ion are

$$\begin{aligned} R_n^{S,Z} = & \sum_{k<n^*} N_e K_{nk}^{S,Z} \left( \bar{N}_k^{S,Z} - \bar{N}_n^{S,Z} \right) \\ & + \sum_{\substack{k>n \\ k<n^*}} \beta_k^{S,Z} A_{kn}^{S,Z} E_{kn}^{S,Z} \bar{N}_k^{S,Z} / \beta_n^{S,Z} \\ & - \bar{N}_n^{S,Z} \left( \sum_{k<n} A_{nk}^{S,Z} E_{nk}^{S,Z} + R_e - \left( \frac{3}{2} + \frac{I_n^{S,Z}}{kT_e} \right) \frac{d \ln T_e}{dt} \right) . \end{aligned}$$

The quasistationary group is  $n^* > n \geq \bar{n}$ . The rate  $(d/dt)N_n^{s,z} = 0$  for this group corresponds to setting  $R_n$ ,  $R_e$  and  $d \ln T_e / dt$  null in the above. Rate equations for all atoms and ions, plus those for cavity intensities (Appendix C) and the electron energy equation for  $d \ln T_e / dt$  together define the model. An implicit assumption in the model is that for any given core, only one excited electron is in a discrete state, the rest being free. The radiative recombination term is given by  $E_{n^*n} \equiv 1$ ,

$$A_{n^*n} = \frac{32}{3\sqrt{3}} \frac{\alpha^3 \text{Ryd}}{h} z^4 \frac{G_n}{p_n^3} N_e \left( \frac{h^2}{2\pi m_e kT_e} \right)^{3/2} \exp\left(\frac{I_{n^*}}{kT_e}\right) F\left(\frac{\Delta E_{n^*}}{kT_e}\right)$$

where  $\alpha$  is the fine structure constant,  $p_n$  the principal quantum number,  $G_n$  the Gaunt factor,  $\Delta E_{n^*n}$  the energy gap to the extended continuum, and  $F(x) \equiv e^{-x} E_1(x)$  [1].

#### Charge and Specie Conservation

The constraints produced by charge and specie conservation are given next. It is assumed that the highest stage of ionization of a specie atom is an ion ground state denoted by  $N_1^s$ . Total specie number density is  $N_s$  and maximum parent charge number is  $z_s$ . Given  $N_s$ ,  $N_1^s$  is found

$$N_s = (1 + \epsilon z_s^{3/2}) N_1^s + N_e (S_a^s + \epsilon S_b^s),$$

$$S_a^s \equiv \sum_{z=1}^{z_s} \sum_{n < n^*} \beta_n^{s,z} \bar{N}_n^{s,z},$$

$$S_b^s \equiv \sum_z (z - 1)^{3/2} \beta_1^{s,z} \bar{N}_1^{s,z}.$$

The terms proportional to  $\epsilon$  give the populations of the bound states parts of the extended continuum. The electron density is obtained using

$$C - \epsilon A = N_e (1 + D - \epsilon B) ,$$

$$S_c^s \equiv \sum_z \sum_n (z - 1) \beta_n^{s,z} \bar{N}_n^{s,z} ,$$

$$S_d^s \equiv \sum_z (z - 2) (z - 1)^{3/2} \beta_1^{s,z} \bar{N}_1^{s,z} ,$$

$$A = \sum_s z_s^{3/2} N_s / (1 + \epsilon z_s^{3/2}) ,$$

$$B = \sum_s \left( S_d^s - z_s S_b^s + z_s^{3/2} (S_a^s + \epsilon S_b^s) / (1 + \epsilon z_s^{3/2}) \right) ,$$

$$C = \sum_s z_s N_s ,$$

$$D = \sum_s (z_s S_a^s - S_c^s)$$

In the above,  $\epsilon$  is calculated with  $N_e = C/(1 + D)$  and then the final value of  $N_e$  is found.

Neglecting terms of order  $\epsilon$ , the conservation and rate equations may be combined to give

$$R_e = \sum_{s,z} (z_s + 1 - z) \left( N_e \alpha_I^{s,z} - N_1^{s,z+1} \alpha_R^{s,z} \right) .$$

$$\alpha_I^{s,z} = \sum_n \beta_n^{s,z} \bar{N}_n^{s,z} K_{nn^*}^{s,z}$$

is an ionization coefficient, and

$$\alpha_R^{s,z} = \sum_n \beta_n^{s,z} \left( N_e K_{nn^*}^{s,z} + \beta_{n^*}^{s,z} A_{n^*n}^{s,z} / \beta_n^{s,z} \right)$$

is a recombination coefficient. Similarly, "rate heating" of the free electron gas D is given as

$$D_e = N_e \sum_{s,z} \left( \bar{N}_1^{s,z+1} d_R^{s,z} - N_e d_I^{s,z} \right),$$

$$d_R^{s,z} = \sum_n \beta_n^{s,z} I_n^{s,z} \left( N_e K_{nn^*}^{s,z} + \beta_{n^*}^{s,z} A_{n^*n}^{s,z} / \beta_n^{s,z} \right)$$

is a recombination heating coefficient and

$$d_I^{s,z} = \sum_n \beta_n^{s,z} I_n^{s,z} \left( \bar{N}_n^{s,z} K_{nn^*}^{s,z} + \sum_{k < n^*} K_{nk}^{s,z} \left( \bar{N}_n^{s,z} - \bar{N}_k^{s,z} \right) \right)$$

is a coefficient of energy absorption for inelastic collisions.

#### Reduction of Rate Equations

The rate equations may be rewritten in the form (for given s,z)

$$R_n = \sum_{k < n^*} M_{nk} \bar{N}_k + F_n \bar{N}_1 +$$

where the + superscript denotes  $z+1$ . Nulling  $R_e$  and  $d\ln T_e/dt$  in matrix  $M$  gives matrix  $M'$ . The rate equations are of the stiff type, i.e., characterized by multiple time scales. Integrators designed to handle this type of problem [4] require the Jacobian matrix  $J_{nm} = \partial R_n / \partial \bar{N}_m$  to scale the numerical integration time step. For the quasistationary levels,  $R_n = 0$  for  $M$  replaced by  $M'$ , giving

$$\bar{N}_j = - \sum_{k,m} M'_{jk}{}^{-1} M'_{km} \bar{N}_m - \bar{N}_1^+ \sum_k M'_{jk}{}^{-1} F_k$$

where  $j, k \geq \bar{n}$  and  $m < \bar{n}$ . Substituting this expression for the quasistationary populations into the rate equations for the lower levels ( $n < \bar{n}$ ) gives the reduced set of equations

$$R_n = \sum_{m < \bar{n}} H_{nm} \bar{N}_m + G_n \bar{N}_1^+$$

where

$$H_{nm} = M_{nm} - \sum_{j,k} M_{nj} M'_{jk}{}^{-1} M'_{km}$$

$$G_n = F_n - \sum_{j,k} M_{nj} M'_{jk}{}^{-1} F_k$$

The Jacobian of the reduced set  $P$  may be found with the aid of the matrix

$$T_{jm} \equiv \partial \bar{N}_j / \partial \bar{N}_m \quad (j \geq \bar{n}, m < \bar{n})$$

Using the chain rule,

$$P_{nm} = J_{nm} + \sum_j J_{nj} T_{jm} \quad (n < \bar{n})$$

and

$$0 = J'_{km} + \sum_j J'_{kj} T_{jm} \quad (k \geq \bar{n}).$$

(Primes have the same significance for J as M.)

Combining,

$$P_{nm} = J_{nm} - \sum_{j,k} J_{nj} J'_{jk}^{-1} J'_{km}$$

where the matrix J is calculated for the quasistationary levels independent. In general, the reduction of the rate equations leads to two matrix inversions.

The dependence of the rates on  $N_e$  and  $\bar{N}_1^+$  leads to cross terms in the reduced Jacobian for different s,z. Due to the algebraic complexity of the model, the Jacobians are formed assuming fixed transition line profiles. The error in this assumption should not be large since the short time scales are associated with upper states which are usually optically thin.

#### Energy Equation and the Penning Effect

The electron energy equation is taken from 13-moment solutions to the Boltzmann equation [1,5]. Included in the equation are the rate of change of enthalpy, elastic electron-heavy particle energy exchange, continuum radiation, collisional-radiative heating  $D_e$ , and joule dissipation. Provision is made in the model to input either the current density or an imposed electric field or to bypass the energy equation by providing the temporal variation of the electron temperature. Heavy particle temperatures are assumed equal and constant.

Due to the possible importance of Penning excitation exchange in lasers having noble gases [6], source code for one and two electron excitation and/or ionization of a receptor atom by a metastable donor is part of the model. This code is placed in blocks for easy removal. The probability of double ionization is apparently small [7].

### Discussion

The model for the laser rate kinetics has been designed to be of a very general nature. The desire for flexibility and to test concepts led to the program form. Atom or ion level structure, oscillator strengths, atomic constants, etc. are input by distinct subprograms that may be changed at will to provide an arbitrary mix of elements and ionization stages. In order that this be done with maximum storage economy, this information is transferred to common blocks on an end-to-end basis. Further flexibility is obtained by the use of Univac Fortran V Parameter variables for dimension information, DO loop constants, index constants and the like. These variables are replaced by their assigned values at compilation. The specification statements for the Parameter variables, array dimensions, etc. are not part of subprogram source code but are placed in Fortran procedures (by the Procedure Definition Processor) for inclusion at compilation. Thus only a single set of source code defining the procedures need be changed before compilation to modify the storage requirements of the assembled program. It is thus possible to minimize storage for a given set of atoms and ions with ease and without error. The numbers of level units in the divers groups can also be readily changed.

The program is designed to treat lower level groups as stiff and Jacobian matrices are calculated. One purpose of the model is to determine if and/or when use of the quasistationary approximation for intermediate groups removes the stiffness so that simpler integrators may be used. Success of this tactic has been recently reported [8], but its use in cases of fast pumping is questionable [1]. Use of the quasistationary group reduces storage requirements; it may or may not help insofar as reducing the program running time. It is necessary to determine the effect on running times and also constraints (e.g. values of

$\bar{n}$  and  $n^*$ ) of the three group model. Another item of consequence is the conditions for an emission factor E of unity. Calculations related to this factor are relatively extensive. After initial calculations, simplifications may ensue.

A detailed listing of the model is provided in Appendix E.

The program is in the process of being debugged. A sample run utilizing a single argon atom only with twelve level units has been apparently successful. Use of multiple species has led to difficulties with the matrix inversion aspect of the program; this anomaly and the configuration of output data remain as program problems. Numerical results will be given in a later report.



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APPENDIX A  
LINE BROADENING

It is desired to have a complete, yet compact, description of the excited states phase shifts (homogeneous broadening) and velocity changes (inhomogeneous broadening). The most rigorous approach is that using the quantum density matrix [9,10]. The need for simplicity in the computer model leads to consideration of classical theory for the estimation of line profiles. In the model line center frequency shifts are neglected and the Voigt integral is used to enfold the Lorentz impact and Doppler profiles. The theory is presented in [11]; results of interest are summarized below.

For an inverse power law potential,  $V = e^2 a_0^{m-1} C_m r^{-m}$ , of emitter-perturber interaction the optical or phase shift cross section is  $\pi b_W^2$  where the Weisskopf radius

$$b_W = \left( \frac{|C_m|}{p_m} \frac{\alpha c}{v} \right)^{\frac{1}{m-1}} a_0$$

The symbols are:  $e$ -electron charge,  $a_0$  - Bohr radius,  $r$  - distance between interacting atoms,  $v$  - relative velocity of atoms,  $c$  - velocity of light,  $\alpha$  - fine structure constant. Constant  $p_m$  is proportional to the critical phase shift that defines the effective interaction range;  $p_3 = 0.318$ ,  $p_4 = 0.411$ ,  $p_6 = 0.533$ ,  $p_{12} = 0.773$ . This impact result is valid for angular frequencies in a region at the line center,  $\Delta\omega < v/b_W$ , and for perturber densities  $N_p$  smaller than  $b_W^{-3}$ . These limits are of small consequence for the problem under discussion. The optical collision frequency (line semi-half width) is  $\pi N_p \langle v b_W^2 \rangle$  where the velocity distribution is taken as Maxwellian. For elastic collisions the phase shifts between the upper and lower states of a line subtract and  $C_m = C_{m(\text{upper})} - C_{m(\text{lower})}$ . In the case of an ion emitter and electron perturbers, a correction for the hyperbolic collision path may be necessary [11]. If  $b_C$  is the Coulomb

collision radius,  $b_C > b_W$ , the cross section increases by a factor of approximately  $2.3(b_C/b_W)^s$ ,  $s = (2m - 4)/(2m - 3)$ , giving an inverse square root dependence of the width on electron temperature. Interactions considered in the model are:

- 1) resonance broadening (ground state atom perturber and like atom emitter),  $|C_3| = 6f_{\text{abs}} \text{Ryd}(g_\ell/g_u)^{1/2}/(\pi\Delta E)$ ; (this interaction involves excitation exchange and is not elastic; the interaction of upper and lower states is added);
- 2) electron-quadrupole broadening,  $|C_3| \approx \langle r_e^2 \rangle_{q_L} / a_0^2$  where  $q_L^2 = \frac{2}{15} L(L+1)/(L(L+1) - 3/4)$  for the emitter;
- 3) electron quadratic Stark broadening,

$$C_4 = 2 \left( \sum_{\text{lower}} f_{\text{ems}} (\text{Ryd}/\Delta E)^2 - \sum_{\text{upper}} f_{\text{abs}} (\text{Ryd}/\Delta E)^2 \right)$$

sums are over all emitter bound states;

- 4) Van der Waals broadening (ground state atom perturber and unlike atom emitter),  $C_6 \approx -\alpha_p \langle r_e^2 \rangle / a_0^5$  ;
- 5) atom perturber and ion quadrupole emitter,  $|C_6| \approx Z \langle r_e^2 \rangle \alpha_p q_L / a_0^5$ .  
(The polarization interaction  $C_4 = -Z\alpha_p / (2a_0^3)$  is state independent and gives no broadening.)

Broadening by ions is small and is neglected. Symbols are:  $f_{\text{ems}}$ ,  $f_{\text{abs}}$  - emission and absorption oscillator strengths, Ryd - Rydberg unit of energy,  $\Delta E$  - transition energy,  $g_\ell, g_u$  - lower and upper degeneracies,  $\langle r_e^2 \rangle$  - average square of the active electron radius of a state,  $L$  - total angular momentum quantum number,  $\alpha_n$  - perturber atom polarizability,  $Z$  - ion charge number.

The parameters in the resonance broadening constant  $C_3$  refer to the transition between the emitter state and the (perturber) ground state. If the emitter state effective principal quantum number  $n > 3$ , the oscillator strength is small and the excitation exchange interaction is weak; further, the emitter radius is large. In this situation, repulsive electron exchange effects become dominant [12]. For  $n \lesssim (\alpha c/v)^{1/4}$ , these effects can be estimated by using  $b_W \approx \langle r_e^2 \rangle^{1/2}$ . Effects at larger  $n$  [12] are not relevant to the model. The maximum of the widths calculated using the two interactions is used.

Broadening by electrons is estimated as the largest of the quadrupole and quadratic Stark interactions. Inelastic collisions between sublevels are frequently important in Stark broadening. Provision is made in the model to calculate the Stark width from curve fits to the calculations of Griem [3], assuming additive upper and lower state interactions. Curve fits of the form  $CN_e n^k T_e^r$  give good results for many levels (typically  $k = 5$  and  $r = 0.4$ ).

The form of the Van der Waals constant  $C_6$  is an approximation valid in the limit of large energy level separations [3,11]. As with the case of resonance broadening, electron exchange effects can be important, especially for small  $\alpha_p$ . Only the simple form above is used; more precise analysis requires involved calculation and more knowledge of potentials than is commonly available. The polarizability  $\alpha_p$  can be found from data [13] or estimated as  $4a_0^3 (\text{Ryd}/\Delta E_r)^2$  where the resonance level-ground energy gap pertains [3]. Also,  $\langle r_e^2 \rangle / a_0^2 \approx n^2(5n^2 + 1 - 3\ell(\ell + 1))/2Z^2$  where  $Z$  refers to the parent ion.

Finally, the total homogeneous line width is the sum of the widths obtained from the formulas above plus that due to the frequencies of quenching of the upper and lower states. The quenching mechanisms are that of spontaneous emission (natural broadening), induced emission or absorption (power broadening) and inelastic excitation and de-excitation between levels ("rate" broadening). Note that the quenching mechanisms give a Lorentz profile without constraint (this includes resonance broadening).

APPENDIX B  
RADIATIVE ESCAPE FACTORS

An escape factor for a given transition gives the effect of induced radiative processes on the emission rate. The factors are calculated assuming a uniform medium and are averaged over the gas volume. For a non-inverted line of large optical depth, trapping gives an escape factor much less than unity. Conversely, amplified spontaneous emission from an inverted line gives an escape factor greater than unity.

The theory of line trapping is discussed in [14-19]. Radiation loss from any particular line may be written as  $N_u h\nu_0 A_{ul} E$  where  $N_u$  is the upper state density,  $h\nu_0$  the line center energy,  $A_{ul}$  the Einstein spontaneous emission coefficient and escape factor  $E = \langle \exp(-\tau_v) \rangle$ ,  $\tau_v$  being the optical depth (negative for an inverted line). The average is taken over frequency and solid angle and for the model also over spatial position. A cylindrical geometry and a Doppler line profile gives  $E = 0.90 / (\tau_0 \sqrt{\ln \tau_0})$  where  $\tau_0$  is the line center optical depth based on the radius. A Lorentz profile gives  $E = 0.63 / \sqrt{\tau_0}$ . Trapping decreases as  $\tau_0$  drops to order unity and for small depth  $E = 1 - \langle \tau_v \rangle$ . In the model, the maximum of the Doppler and Lorentz factors (large  $\tau_0$  limit, each calculated using the appropriate limiting line profile) is used to approximate trapping for the Voigt profile; then a smooth interpolation to the small depth limit is performed so that the entire range of optical parameters is covered in a convenient yet reasonable manner. Note that at large depths, escape is determined by the line wings where the homogeneous broadening dominates since it is of distinct proportion. The approximation used gives negligible error at the larger optical depths where trapping is most pronounced. (Some error may occur due to non-impact optical interactions not properly accounted for in the model; the effect of this is considered slight since it can manifest itself only in cases of near complete trapping, i.e., at small optical transition rates.)

An interpolation scheme between small and large gain limits is also used for inverted transitions. A discussion on the calculation of  $\langle \exp(|\tau_v|) \rangle$  for  $|\tau_v| \gtrsim 1$  follows. Let the cylinder center line optical depth value for the transition line center be  $g$ ,  $L$  the cylinder length (which defines  $g$ ),  $R$  the cylinder

radius,  $r$  the distance from an emission point to a cylinder boundary point,  $\bar{p}(v)$  the line profile relative to the line center  $v_0$  so that  $\bar{p}(v_0) = 1$ , and the cylinder aspect ratio  $b = L/(2R)$ . Then  $E = \langle \exp(g\bar{p}r/L) \rangle$ . Averaging over frequency,  $E = \langle F(gr/L) \rangle$  where

$$F(s) = \frac{k}{\sqrt{\pi}} \int_{-\infty}^{\infty} \bar{p}(x) \exp(s \bar{p}(x)) dx,$$

$k \equiv \sqrt{\pi} w_v p_0$ :  $w_v$  the Voigt half-width and  $p_0$  the line center absorption coefficient,  $x \equiv (v - v_0)/w_v$ . For a Lorentz profile  $\bar{p} = (1 + x^2)^{-1}$ ,  $F(s) = \sqrt{\pi} k \exp(s/2) I_0(s/2) \approx k \exp(s)/\sqrt{s}$  for large  $s$ . For a Doppler profile,  $\bar{p} = \exp(-x^2)$  and it can be easily shown that  $F$  approaches the same limit for large  $s$ . Since  $F(0) = 1$ , the large gain limit is calculated using  $F(s) \approx 1 + k(e^s - 1)/\sqrt{s}$ . In the Lorentz limit, this approximation gives a relative error  $\leq 20\%$  for  $0 < s \leq 1$ ,  $\leq 5\%$  for  $s \geq 2$ . In the Doppler limit, the error is as large as 34% at smaller  $s$ . The similar results for the profile limits is to be expected since it is the line center that controls the amplification process.

Let the cylinder center line be parallel to the  $z$ -axis in rectangular coordinates, offset in the  $x$  direction by amount  $\omega R$ ,  $0 \leq \omega \leq 1$ . The equations for the cylinder wall are

$$x = 2R q \cos \theta$$

$$y = 2R q \sin \theta$$

$$q \equiv \frac{1}{2} \left( \omega \cos \theta + (1 - \omega^2 \sin^2 \theta)^{1/2} \right)$$

$$z = r \cos \phi, \quad 2Rq = r \sin \phi$$

Consider  $0 \leq z \leq vL$ ,  $0 \leq v \leq 1$ ; then for the cylinder side  $\phi_0 \leq \phi \leq \frac{\pi}{2}$  where  $q \cot \phi_0 = b v$ . The solid angle differential is  $\sin \phi d\phi d\theta$ . The emitter position is characterized by the variables  $v$  and  $\omega$ ; the volume average is given by

integration over  $2 \omega d\omega d\theta$ . For  $H(s) = (\exp(s) - 1)/\sqrt{s}$ , the excess side loss  $E_{es} = (E - 1)_{side}$  is approximately

$$E_{es} = \frac{2k}{\pi} \int_0^1 \omega d\omega \int_0^\pi d\theta \int_0^1 d\upsilon \int_{\phi_0}^{\pi/2} \sin \phi d\phi H\left(\frac{gq}{b \sin \phi}\right).$$

The integrals over  $\omega$  and  $\theta$  can be transformed to a single integral over  $q$  and the integrals over  $\upsilon$  and  $\phi$  can be transformed to a single integral by integration by parts. Using  $u \equiv gq/b$ , the result is

$$E_{es} = \frac{4kb}{\pi g} \int_0^{g/b} u^2 du \sqrt{1 - (bu/g)^2} \int_u^{\sqrt{u^2+g^2}} H(s) \frac{ds}{s^2} \left( \frac{1}{\sqrt{s^2 - u^2}} - \frac{1}{g} \right).$$

After removing the singularity at  $s = u$  by integration by parts, the remaining integration is done numerically. The results are given in Figure B1. It is seen that  $E_{es}$  is significant only for  $g \gtrsim b$ , corresponding to large transverse gain. For the low gain limit  $E_{es} = \langle |\tau_\nu| \rangle_{side}$ , or  $E_{es} = g \langle \bar{p}(\nu) \rangle \langle r/L \rangle_{side}$ . The last factor is

$$\langle r/L \rangle_{side} = \frac{4}{\pi b^2} \int_0^1 q^2 dq \sqrt{1 - q^2} \left( \frac{b}{q} \tan^{-1} \frac{b}{q} - \frac{1}{2} \ln \left[ 1 + \left( \frac{b}{q} \right)^2 \right] \right).$$

After numerical evaluation for  $b > 1$ , the following curve fit gives this factor with an error less than 1%:

$$\langle r/L \rangle_{side} \doteq 0.66/b - 1.09/b^2 + 2.30/b^3 - 1.60/b^4.$$

The average solid angle that the side subtends is  $4\pi S_s$  where

$$S_s = \frac{4}{\pi b} \int_0^1 dq \sqrt{1 - q^2} (\sqrt{q^2 + b^2} - q) \doteq 1 - 0.4244/b + 0.172/b^2 - 0.090/b^3 + 0.025/b^4.$$



If  $a$  is the ratio of the Lorentz half-width to Doppler width, then

$$k \doteq (1 + 0.7304a + 0.5811a^2)/(1 + 1.2946a + 1.0299a^2)$$

and

$$\langle \bar{p} \rangle \doteq (0.707 + 1.25a)/(1 + 2.5a) \text{ within an error of 2.3\%}$$

Similar calculations apply to the cylinder ends:

$$E_{ee} = \frac{2kg}{\pi b^2} \int_0^1 q dq (\cos^{-1} q - q \sqrt{1 - q^2}) \int_u^{\sqrt{u^2 + g^2}} H(s) \frac{ds}{s^2},$$

and

$$\begin{aligned} \langle r/L \rangle_{\text{ends}} &= \frac{1}{\pi b^2} \int_0^1 q dq (\cos^{-1} q - q \sqrt{1 - q^2}) \ln \left[ 1 + \left( \frac{b}{q} \right)^2 \right] \\ &\doteq (0.9428 + \ln b)/(8b^2) + 0.0132/b^4. \end{aligned}$$

Results of numerical calculation of the excess end loss  $E_{ee}$  are given in Figure B2.

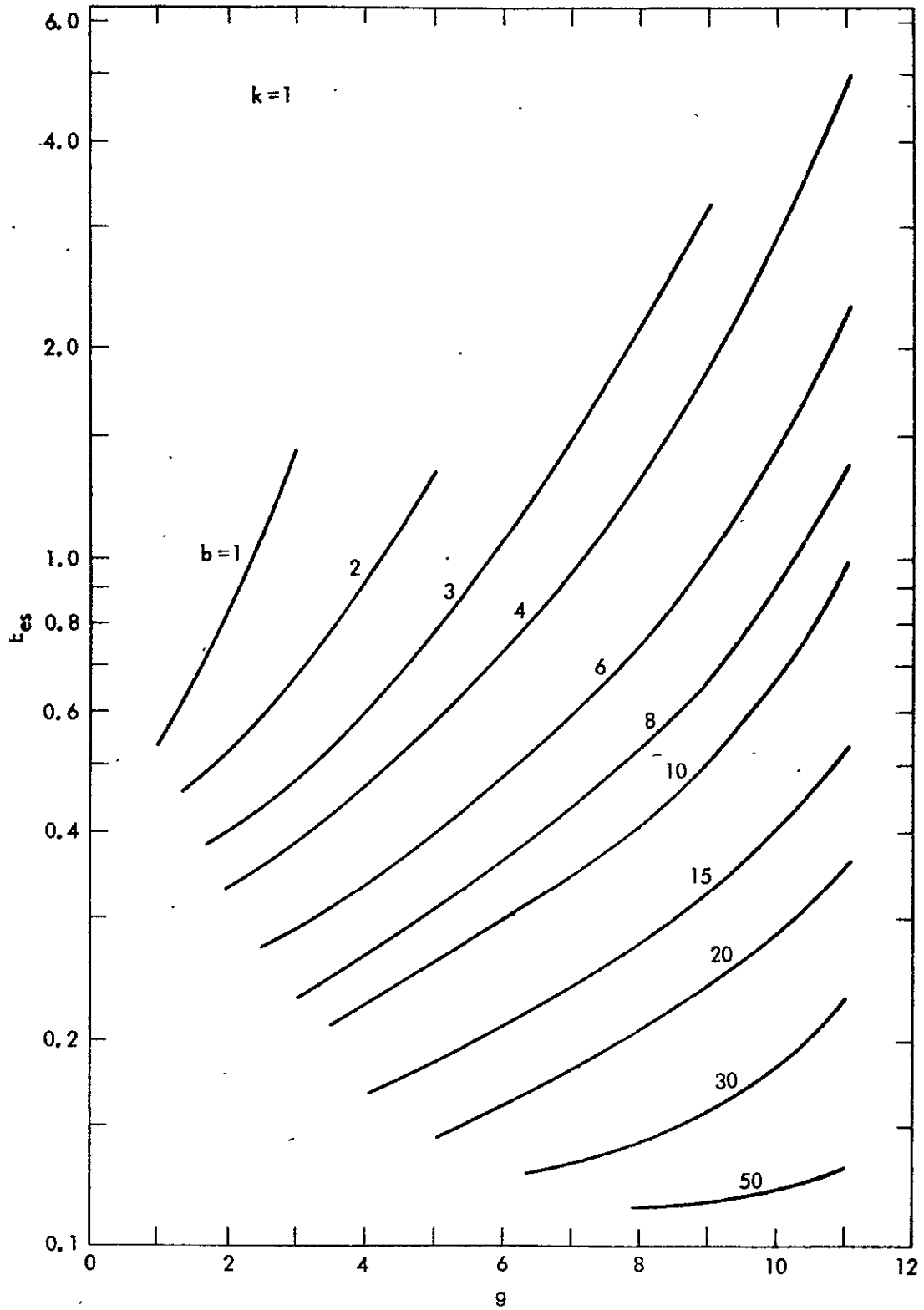


Fig. B1. Excess side emission factor for inverted transitions as a function of axial gain. Parameter  $b$  is the cavity aspect ratio.

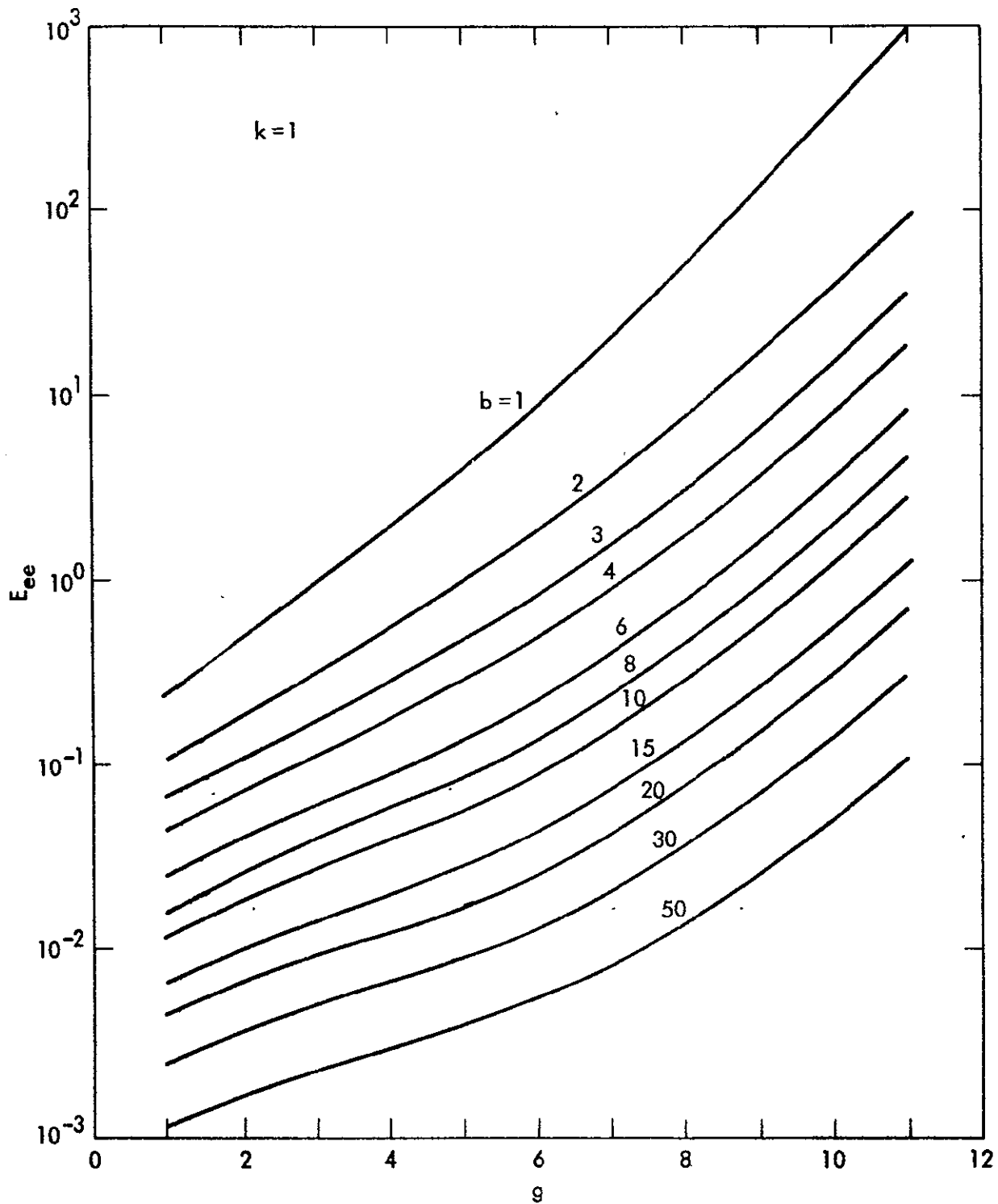


Fig. B2. Excess end emission factor for inverted transitions as a function of axial gain. Parameter  $b$  is the cavity aspect ratio.

APPENDIX C  
CAVITY EQUATIONS

Quantum coherency effects are not considered in the modeling of the interaction of strong cavity electromagnetic fields with atomic excited state populations. Feedback from the optical cavity and saturation effects are estimated using rate type equations with steady state intensity profiles without velocity distribution or spatial hole burning. The present form of the cavity equations contain inherent inaccuracies that would be most pronounced for low pressure and/or very fast developing systems. This situation is dictated by the need for relative overall simplicity; future simplifications in other aspects of the model may lead to further development of the cavity equations.

Denote the total intensity for a given transition as  $I = ch\nu_o N_{ph}$  where  $N_{ph}$  is the photon density. The corresponding spectral quantities are  $I_\nu = ch\nu N_\nu$ . For each direction of propagation,

$$\frac{dN_\nu}{dt} = \frac{c^3}{8\pi\nu^2} A_{u\ell} p(\nu) (N_u - g_u N_\ell / g_\ell) N_\nu + \eta A_{u\ell} N_u - N_\nu / t_c,$$

$A$  is the Einstein emission coefficient,  $p$  the transition profile,  $\eta$  the solid angle and polarization factor, and the cavity decay time  $t_c = L / (c \ln(1/\sqrt{R_1 R_2}))$  for length  $L$  and mirror reflectivities  $R_1$  and  $R_2$ . The intensity is taken unpolarized and  $\nu$  replaced by  $\nu_o$  except in the profile functions. (For plane polarized light,  $\eta \rightarrow \eta/2$ .) Let the line center gain logarithm be

$$g = \frac{A_{u\ell}}{8\pi} \left( \frac{c}{\nu_o} \right)^2 (N_u - g_u N_\ell / g_\ell) L p_o,$$

$\Delta\nu$  the mode spacing, and the saturation parameter  $s \equiv g / \ln(1/\sqrt{R_1 R_2})$ . Then summing over modes (frequencies):

$$\frac{dN_{ph}}{dt} = (ws - 1) N_{ph} / t_c + \eta_e A_{u\ell} N_u$$

where for mode intensities  $I_m$ ,

$$\omega = \sum_m I_m p(v_m) / I p_0$$

and

$$n_e = \sum_m n(v_m) \Delta v = \int n dv$$

defines the total spontaneous emission noise into all active modes. Note that

$$I = \sum_m I_m$$

and  $\omega \leq 1$ . The mode spacing  $\Delta v = cf/(4L)$  where the cavity length and mirror radii define  $f$ . For the model,  $f = (x/(2-x))^{1/2}$ ,  $0 < x < 2$ ,  $x$  is the ratio of length  $L$  to the effective mean mirror radius. (This equation defines the mean radius.) Only one mode exists if  $p_0 \Delta v \gtrsim 1$ . The intensity profile-transition profile overlap integral  $\omega$  is approximated by using steady state saturation intensity expressions. For homogeneous broadening a set of longitudinal modes gives [20]:

$$\omega(s) = \left[ 1 - \coth\left(\frac{1}{p_0 \Delta v}\right) \tanh\left(\frac{\sqrt{1-s}}{p_0 \Delta v}\right) \sqrt{1-s} \right] / s$$

As  $s \rightarrow 1$  (or  $p_0 \Delta v \rightarrow \infty$ ),  $\omega \rightarrow 1$ . This narrowing effect of saturation can be generalized by considering an intensity profile of the form  $\bar{p}(v)/(1 - s\bar{p}(v))$ . Then in the limit  $s \rightarrow 0$ ,  $\omega \rightarrow \langle \bar{p} \rangle$  (a function of the ratio of Lorentz to Doppler widths, Appendix B). Numerical integration is performed to find  $\omega$  in the limit  $p_0 \Delta v \rightarrow 0$ , a curve fit to the results is modified for finite  $p_0 \Delta v$  to give

$$\omega(s) \approx 1 - (1-s)^{0.3} (1 - \langle \bar{p} \rangle) / (1 + p_0 \Delta v)$$

This is the generalized saturation narrowing used in the model.

The present cavity model can be expected to be a valid approximation at higher pressures where impact broadening is significant and at inversions not many times that at threshold. Different transverse modes have different diffraction losses; the number of modes taken must be equal to those of relatively small loss. This number would define the effective emission solid angle  $\eta_e$ . It must depend on the number of photon passes in the cavity, cavity geometry, wavelength, and transition width. At present the parameter  $\eta_e$  is input into the program. The single mode minimum value is  $(\lambda/(2\pi R))^2$ ; an upper bound is the average end solid angle (Appendix B). Spontaneous emission noise is most important at the start of the intensity buildup and the larger values of  $\eta_e$  are most pertinent.

The model presents the maximal effect of saturation narrowing within the rate approximation; calculations with  $\omega(s \equiv 0)$  may be used to determine the minimal effect.

## APPENDIX D

## CLASSICAL EXCITATION RATES

Expressions are needed for excitation rates between many pairs of levels. The expressions must be general in nature and relatively simple, yet reasonably accurate. The use of classical theory produces expressions that satisfy these constraints [1]. Provision is made in the model to use empirical excitation rates from ground states.

The present model utilizes the cross sections of Gryzinski [21]. Excitation from a level "l" to all levels "u" and above (including the continuum states) is given by the coefficient [22]:

$$\bar{K}_{lu}(T_e) = g_e R(y, A) / \Delta E_{lu}^{3/2},$$

where  $g_e$  is the number of equivalent electrons in the lower state,  $\Delta E_{lu}$  is the energy gap,  $y \equiv \Delta E_{lu} / kT_e$ ,  $A \equiv I_l / \Delta E_{lu} \geq 1$  for lower state ionization energy  $I_l$ . The rate coefficient to level "u" alone is obtained by subtracting a similar expression with  $u \rightarrow u + 1$ :  $K_{lu} = \bar{K}_{lu} - \bar{K}_{lu+1}$ . Ionization is given by  $\bar{K}$  with  $A \equiv 1$ . For  $A \leq 10$  and  $0.01 \leq y \leq 10$ , a good analytical approximation to numerical evaluation of rate coefficients using a Maxwellian velocity distribution is [22]:

$$R = (3.84 \times 10^{-6} \text{ cm}^3 \text{ eV}^{3/2} \text{ sec}^{-1}) y^t e^{-y} / \left( A^{1/4} (y^2 + 7y/4 + 1/9) \right),$$

$$t = (A + 30) / (10A + 25).$$

Asymptotic expansions for small and large  $y$  yield respectively

$$R(y \text{ small}) = 4.39 \times 10^{-6} \sqrt{y} e^{-y} \left( 1 - A \ln(Ay) / 3 \right),$$

$$R(y \text{ large}) = 2.93 \times 10^{-6} e^{-y} / (\sqrt{A} y^S), \quad S = (3A + 1) / (2A + 2).$$

These functions are suitably matched in the intermediate regions. The above excitation function may be applied to allowed transitions. Gryzinski's exchange

cross sections give coefficients for forbidden transitions; a curve fit is made to numerical calculations [23].

Another classical calculation is that of Mansbach and Keck [24], where Monte Carlo trajectories are used in a three body (free electron, active electron, parent ion) system. For principal quantum numbers  $n_\ell$  and  $n_u$ , excitation rate coefficient

$$K_{\ell u}(T_e) = 3.73 \times 10^{-7} \text{ cm}^3 \text{ sec}^{-1} \left( \frac{\text{Ryd}}{kT_e} \right)^{0.17} \frac{n_\ell^{4.66}}{n_u^3} e^{-y}$$

and for ionization

$$K_{\ell\infty}(T_e) = 1.87 \times 10^{-7} \text{ cm}^3 \text{ sec}^{-1} \left( \frac{kT_e}{\text{Ryd}} \right)^{0.83} n_\ell^{4.66} e^{-Ay} .$$

(Calculations are made for hydrogen-like atoms.) These rates are smaller than that of Gryzinski for small energy gaps,  $\Delta E \lesssim kT_e$  [24]. Since coefficients are large under this condition and the levels involved tend to be quasi-stationary [1], the difference is probably of small significance. Within the classical approximation, the Mansbach-Keck rates may be regarded as theoretically more rigorous. However, collective interactions between free electrons and a highly excited active electron make the accuracy of any lone perturber collision theory doubtful for transitions between levels of large quantum number. The model may be easily modified to employ Mansbach-Keck or quantum Born excitation rates.

The form of the excitation coefficient as given by the R-function can be expected to be approximately correct for ions as well as atoms [25].



APPENDIX E  
PROGRAM LISTING

The computer program is written in terms of the following units or reference values for physical quantities.

pressure	1 mbar = $10^2 \text{ Nm}^{-2} \approx 10^{-3} \text{ atm}$
density	$10^{15} \text{ cm}^{-3}$
rate coefficient	$10^{-7} \text{ cm}^3 \text{ sec}^{-1}$ (also Stark coefficient)
line width, relaxation time	$10^8 \text{ sec}^{-1}$
temperature	$10^4 \text{ }^\circ\text{K}$
atomic mass	1 amu = $1.66053 \times 10^{-27} \text{ kg}$
length (except wavelength)	1 cm
wavelength	1 $\mu\text{m}$
elastic cross section	$10^{-15} \text{ cm}^2$
current density	1 abamp $\text{cm}^{-2} = 10^5 \text{ amp m}^{-2}$
electric conductivity	1 mho $\text{cm}^{-1}$
electric field	1 kV $\text{m}^{-1}$
magnetic field	1 web $\text{m}^{-2}$
intensity	1 W $\text{cm}^{-2}$

The following symbol conventions are used generally throughout the program. The few exceptions are noted later.

AN	vector of ground state populations $N_1^{s,z}$ of atom or ion type s,z
ANB	vector of normal excited state populations $\bar{N}_n^{s,z}$
ANC	vector of specie densities $N_s$
ANE	electron density $N_e$
ANP	vector of densities of maximum ionization $N_1^s$
CAR	laser cavity aspect ratio b
CL	cavity cylinder length
CMR	cavity mean mirror reflectivity $\sqrt{R_1 R_2}$
NBAR	vector of level indices $\bar{n}$
NCM	maximum number of species (distinct nuclear cores)
NSP	number of atom and ion types

NSTAR    vector of level indices n\*  
 T        heavy particle temperature  
 TE       electron temperature  
 Z or ZC   charge number z of parent ion  
 ZS       maximum charge number z<sub>g</sub> of specie

In the Fortran procedure source deck SPECS, values of Parameter variables are to satisfy the constraints:

If

$NL_k \equiv$  maximum number of level units of atom or ion type k as given by the data input subprograms,

$KM \equiv$  maximum number of equations to be integrated,

Then

$$NLM \geq \max (NL_k) ,$$

$$ND \geq \sum_k NL_k ,$$

$$M \geq 1 + NSP + \sum_k (NL_k + 3)^2$$

$$NT \geq \max \left( (NLM + 3)^2, NLM^2 + NLM + 20 \right) ,$$

$$KSV \geq 1 + 3 NLM + 5 NLM^2/4 .$$

In the format specifications in procedure SPEC3, the second record of format 62 and the third record of format 63 refer to the vector ANC and must have data length equal to NCM; the third and fourth record of 62 and the fourth record of 63 refer to vectors NBAR, NSTAR with data lengths determined by NSP. The program is written for a maximum of four cavity equations. This is reflected in the

last dimension of ICAV, the dimension of WL, the last record of format 62 and corresponding last record of 63 referring to ICAV, the last dimensions of GP and LU in SPEC4 and the dimension of ANPH in SPEC7. Symbols in the procedures are defined in this appendix as the need arises. Common blocks LEVELS, EESND and PENCOM are used for input data and calculated primary variables, TEMPS, INCR, STORE and MSTOR are used for scratch and data transfer between subroutines.

Along with the proper specification statements, a particular problem requires that appropriate data and function subroutines be included in the program assembly. These subroutines are described in succeeding pages. Their specific names are required by the Collector for substitution in dummy subroutine calls. The proper Collector directives are essential to a problem.

-PDP, IFL SPECS

SPEC1 PROC

```

PARAMETER NSP=3,M=1591,ND= 60,NLM=20,NT=529,NPL=NLM+1,NSQ=NLM*NLM,
C   MB=4*ND
DIMENSION DS(M),INDS(M),INX(NSP,8),BP(MB),TMP(NT)
COMMON/LEVELS/INX,DS,BP/TEMPS/TMP
EQUIVALENCE (DS,INDS)

```

END

SPEC2 PROC

```

PARAMETER NCM=3
DIMENSION IC(NCM),ANC(NCM),ANB(ND),NBAR(NSP),NSTAR(NSP),ICAV(3,4):
C   CFST(4),BT(ND),WL(4)
COMMON/EESND/IC,NC,NBAR,NSTAR,ICAV,NCAV,CL,CAR,CMR,ETA,FCAV,CGM,
C   PS,CFST,TE,T,ANE,ANC,ANB,BT,WL

```

END

SPEC3 PROC

```

62  FORMAT(1P8E10.3/1P3E10.3/3I3/3I3/12I3)
63  FORMAT(1H1,2X14HCAVITY LENGTH=1PE10.3,2X16HLENGTH/DIAMETER=
C   1PE10.3,2X13HMIRROR REFL.=1PE10.3,2X11HMODE RATIO=1PE10.3,
C   2X11HRES. RATIO=1PE10.3/
C   3X3HTE=1PE10.3,2X2HT=1PE10.3,2X3HNE=1PE10.3/
C   3X3HNC=3(2X1PE10.3)/
C   3X5HNBAR=3(2X13),2X6HNSTAR=3(2X13)/
C   3X16HCAVITY INDICES= 4(2X3I3) )

```

END

SPEC4 PROC

```

PARAMETER NHSQ=(NLM+NSQ)/2,NP4=NHSQ+21
DIMENSION AN(NSP),w(NHSQ),WD(NHSQ),PHI(NHSQ),R(ND),
C   GP(3,4),LU(2,4)
COMMON/INCR/R
EQUIVALENCE (WD(1),TMP(21)),(WD(1),PHI(1)),(W(1),TMP(NP4)),
C   (GP(1,1),TMP(1)),(LU(1,1),TMP(13))
IFN(I,L)=((I-1)*(2*L-1))/2

```

END

SPEC5 PROC

```

LOGICAL LPN
COMMON/PENCUM/LPN,RPEN,JRC,JRL,JDC,JDL

```

END

SPEC6 PROC

```

PARAMETER KSV= 561
DIMENSION SV(KSV)
COMMON/STORE/SV

```

END

SPEC7 PROC

```

PARAMETER KM=50,NRSTM=2*NLM*NLM+KM*KM+3*(NLM+KM)
DIMENSION ANR(KM),ANPH(4),STRMTX(NRSTM)
COMMON/MSTOR/STRMTX

```

END

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Subroutine DATAIN is used to input and collect the data defining the particular problem at hand. The dummy calls LDUMYn are made equivalent to the names of the atom and ion data subroutines used in the problem by the Collector processor which generates the executable absolute program. It is assumed  $NSP \leq 6$ . The argument list in the data subroutines is as follows:

PQ	vector effective principal quantum numbers based on term values
AQ	vector angular momentum quantum numbers (active electron)
AQT	vector total angular momentum quantum numbers
DG	vector degeneracies
ID	integer vector with the properties: ID(1) is the number of ground level equivalent electrons; otherwise, nominal ID(j) = 1, ID(j) < 0 if the Stark broadening of level j is to be calculated by the curve fit to Griem's tables (Appendix A),  ID(j)  = 2 if empirical excitation rates from the the ground level to j are to be used
W	vector Gaunt factor for radiative recombination into levels [1]
FR	array of transition oscillator strengths, these are input $\leq 0$ for nonallowed transitions (array is two dimensional)
NL	dimension of arrays, i.e., maximum number of levels
GCLI	degeneracy of ground level of next ionization stage
GFF	overall Gaunt factor for recombination radiation,

$$= \frac{5}{6} \sum_{j < n^*} \omega_j G_j p_j^{-3}$$

for  $p_j \equiv PQ(j)$ ,

$\omega_j$  is the relative weight of level j in its shell, and for hydrogenic levels the shell Gaunt factor

$$G_j = 1 - 0.173p_j^{-2/3} - 0.050p_j^{-4/3}$$

IS                    integer parent ion charge number  
 AM                    atomic mass  
 ALPHA                polarizability (applies to atoms only, null for ions)  
 CS, RS, KS          Stark curve fit parameters (Appendix A)

The calls place data into temporary storage TMP, then a call to TRANS shifts the data into the array DS (INDS).  $DS(1) = NSP$ ,  $DS(k + 1) = NL_k$  ( $1 \leq k \leq NSP$ ). The array INX(k, i) contains storage locations of the first elements of arrays for type k according to i=1: array is (IS, AM, GNLI, GFF, ALPHA, CS, RS, KS), i=2: PQ, i=3: AQ, i=4: AQT, i=5: DG, i=6: ID, i=7: W and i=8: FR. The oscillator strength for a transition  $m \rightarrow n$

$$|FR(m,n)| = |DS(m - 1 + NL_k * (n - 1) + INX(k, 8))| .$$

For level units made from levels of different momentum quantum numbers  $\ell$ , the average of the product  $\ell(\ell + 1)$  is used to determine AQ(j). For each type k, a set of four vectors of broadening parameters is placed sequentially into the array BP. The first vector is the resonance broadening constant  $C_3$ , the second vector  $\langle r_e^2 \rangle / a_0^2$ , the third vector Stark constant  $C_4$  and the fourth vector the sum of A-values to lower levels, i.e., the natural line width (Appendix A). Functions F1 and F2 are used to complete the sums over levels in  $C_4$  for  $j \geq n^*$ . These functions are based on hydrogenic oscillator strengths. The vector IC gives the type index for atoms of the species and NC is the number of species.

Array ICAV inputs the transitions that are to be considered in the cavity equations. The first index of ICAV indicates the following: 1 for type index (or null), 2 for lower level index and 3 for upper level index. NCAV is the number of cavity equations. Symbol ETA is the effective noise emission factor for the cavity and CGM is the ratio of the length to effective mean mirror radius (Appendix C). The subroutine changes CGM to the mode spacing and calculates the cavity decay rate as FCAV, the number of photon passes as PS and the wavelengths as WL.

The dummy call to SDUMMY is to be replaced by the Collector by EQUIL or QSTAT which initialize the level populations according to equilibrium or quasistationary

calculations respectively. These subroutines are discussed later; they place the Saha factors in the vector BT.

The Penning effect inputs into PENCOM are logical constant LPN - true if the effect is to be considered, RPEN - Penning rate constant (negative for two electron excitation), JRC - receptor specie index, JRL - receptor level index, JDC - donor specie index and JDL - donor level index. The donor specie must follow the receptor specie at data input.

Subroutine DATAIN and corollary subroutines may be placed in a separate segment in the absolute program since they are needed only at the program start. Thus they do not represent any added storage in the program.

```

-TFOR,SI  SUB1
  SUBROUTINE DATAIN
  INCLUDE SPEC1,LIST
  INCLUDE SPEC2,LIST
  INCLUDE SPEC3,LIST
  INCLUDE SPEC5,LIST
  INCLUDE SPEC7,LIST
  PARAMETER N1S1=NPL+9,N1S2=N1S1+NLM,N1S3=N1S2+NLM,N1S4=N1S3+NLM,
  C    N1S5=N1S4+NLM,N1S6=N1S5+NLM
  DIMENSION PQ(NPL),AQ(NLM),AQT(NLM),DG(NLM),ID(NLM),W(NLM),FR(NSQ)
  DIMENSION R(ND)
  COMMON/INCR/R
  EQUIVALENCE (IS,TMP(1)),(AM,TMP(2)),(GNLI,TMP(3)),(GFF,TMP(4)),
  C    (ALPHA,TMP(5)),(CS,TMP(6)),(RS,TMP(7)),(KS,TMP(8)),(PQ(1),
  C    TMP(9)),(AQ(1),TMP(N1S1)),(AQT(1),TMP(N1S2)),(DG(1),
  C    TMP(N1S3)),(ID(1),TMP(N1S4)),(W(1),TMP(N1S5)),
  C    (FR(1),TMP(N1S6)),(JS,NSTRT),(ANR(1),STRMTX(1)),
  C    (ANPH(1),STRMTX(1))
110  FORMAT(L7,1PE10.3,4I3)
111  FORMAT(1HU,2X23HPENNING RATE CONSTANT =1PE10.3,5X10HRCPT CORE I3,
  C 5X11HRCPT LEVEL I3,5X9HDNR CORE I3,5X10HDNR LEVEL I3)
  F1(X,Y)=1.0/(1.0-X*X/(Y*(Y-1.0)))**4-1.0
  F2(X,Y)=0.49*X**3*(1.0-2.8*EXP(-1.4*AMAX1(Y-X,0.75)))*
  C    F1(X,X+AMAX1(Y-X,0.75))
  INDS(1)=NSP
  NSTRT=NSP+2
  L=1
  C  DUMMY SUBR CALLS ARE TO BE CONVERTED BY COLLECTOR
  CALL LDUMY1(PQ,AQ,AQT,DG,ID,W,FR,NL,GNLI,GFF,IS,AM,ALPHA,CS,RS,KS)
  IF(L.GT.NSP.OR.NSTRT.GT.M-8-6*NL-NL*NL) GO TO 40
  CALL TRANS
  IF(NSP.EQ.1) GO TO 5
  CALL LDUMY2(PQ,AQ,AQT,DG,ID,W,FR,NL,GNLI,GFF,IS,AM,ALPHA,CS,RS,KS)
  IF(L.GT.NSP.OR.NSTRT.GT.M-8-6*NL-NL*NL) GO TO 40
  CALL TRANS
  IF(NSP.EQ.2) GO TO 5
  CALL LDUMY3(PQ,AQ,AQT,DG,ID,W,FR,NL,GNLI,GFF,IS,AM,ALPHA,CS,RS,KS)
  IF(L.GT.NSP.OR.NSTRT.GT.M-8-6*NL-NL*NL) GO TO 40
  CALL TRANS
  IF(NSP.EQ.3) GO TO 5
  CALL LDUMY4(PQ,AQ,AQT,DG,ID,W,FR,NL,GNLI,GFF,IS,AM,ALPHA,CS,RS,KS)
  IF(L.GT.NSP.OR.NSTRT.GT.M-8-6*NL-NL*NL) GO TO 40
  CALL TRANS
  IF(NSP.EQ.4) GO TO 5
  CALL LDUMY5(PQ,AQ,AQT,DG,ID,W,FR,NL,GNLI,GFF,IS,AM,ALPHA,CS,RS,KS)
  IF(L.GT.NSP.OR.NSTRT.GT.M-8-6*NL-NL*NL) GO TO 40
  CALL TRANS
  IF(NSP.EQ.5) GO TO 5
  CALL LDUMY6(PQ,AQ,AQT,DG,ID,W,FR,NL,GNLI,GFF,IS,AM,ALPHA,CS,RS,KS)
  IF(L.GT.NSP.OR.NSTRT.GT.M-8-6*NL-NL*NL) GO TO 40
  CALL TRANS
  JS=0
  DO 30 K=1,NSP
  L=INDS(K+1)
  L1=INX(K,3)-1
  L2=INX(K,2)-1
  L3=INX(K,5)
  L4=INX(K,8)-L
  Z=INDS(L2-7)**2

```

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DO 20 I=1,L
A= Z/DS(L2+1)**2- Z/DS(I+L2)**2
IF(I.EQ.1) A=1.0E9
B=SQRT(DS(L3)/DS(I+L3-1))
BP(I+JS)=1.91*B*ABS(DS(I*L+L4))/A
A=DS(I+L2)**2
B=1.0-3.0*DS(I+L1)*(1.0+DS(I+L1))
BP(I+JS+L)=A*(5.0*A+B)/(2.0*Z)
B=0.0
C=0.0
DO 10 J=1,L
A= Z/DS(J+L2)**2- Z/DS(I+L2)**2
IF(I.EQ.J) A=1.0E5
A=SIGN(A*A,A)
IF(I.GT.J) C=C+A*ABS(DS(I+L*J+L4-1))
10 B=B+2.0*ABS(DS(I+L*J+L4-1))/A
B=B-F2(DS(I+L2),DS(L1))
BP(I+JS+2*L)=B
20 BP(I+JS+3*L)=6.39*C
JS=JS+4*L
30 CONTINUE
GO TO 50
40 WRITE(6,42)
42 FORMAT(1H0,3X20HINCORRECT INPUT DATA)
STOP
50 JS=0
DO 60 K=1,NSP
L=INX(K,1)
L=INDS(L)
IF(L.NE.1) GO TO 60
JS=JS+1
IF(JS.GT.NCM) GO TO 40
IC(JS)=K
60 CONTINUE
NC=JS
READ(5,62) CL,CAR,CMR,ETA,CGM,TE,T,ANE,ANC,NBAR,NSTAR,ICAV
DO 66 K=1,ND
66 R(K)=0.0
NCAV=0
DO 70 K=1,4
70 IF(ICAV(1,K).GT.0) NCAV=NCAV+1
DO 80 K=1,NSP
IF(NSTAR(K).GT.(INDS(K+1)+1)) NSTAR(K)=INDS(K+1)+1
80 IF(NBAR(K).GT.NSTAR(K)) NBAR(K)=NSTAR(K)
DUMMY SUBR CALLS ARE TO BE CONVERTED BY COLLECTOR
CALL SDJMY
WRITE(6,63) CL,CAR,CMR,ETA,CGM,TE,T,ANE,ANC,NBAR,NSTAR,ICAV
A=TVEF(1.0,CAR,1.0)
IF(ABS(CGM-1.0).GE.1.0.OR.CMR.GT.1.0.OR.CMR.LE.0.0) GO TO 40
CFST(1)=CSA(CAR,0)
CFST(2)=CSA(CAR,1)
CFST(3)=CSA(CAR,2)
CFST(4)=CSA(CAR,3)
READ(5,110) LPN,RPEN,JRC,JRL,JDC,JDL
IF(.NOT.LPN) GO TO 96
IF(ABS(RPEN).GT.0.0) GO TO 90
LPN=.FALSE.
GO TO 96
90 K=IC(JRC)

```

```

IF(RPEN.LT.0.0) GO TO 92
IF(JRL.GT.NSTAR(K)) JRL=NSTAR(K)
GO TO 94
92 IF(K.EQ.NSP) GO TO 94
IF(JRL.GT.NSTAR(K+1)) JRL=NSTAR(K+1)
94 WRITE(6,11) RPEN,JRC,JRL,JDC,JDL
IF(JRC.GE.JDC) GO TO 40
IF(JDC.GT.NC) GO TO 40
K=IC(JDC)
IF(JDL.GE.NSTAR(K)) GO TO 40
96 FCAV=299.7925*ALOG(1.0/CMR)/CL
CGM=SQRT(CGM/(2.0-CGM))
CGM=74.948*CGM/CL
PS=1.0/ALOG(1.0/CMR)
IF(NCAV.LE.0) GO TO 98
DO 97 J=1,NCAV
K=ICAV(1,J)
L=INX(K,1)
C=INDS(L)**2
L=INX(K,2)-1
I=ICAV(2,J)
K=ICAV(3,J)
A=C/DS(I+L)**2-C/DS(K+L)**2
97 WL(J)=9.11267E-2/A
98 L=0
DO 100 K=1,NSP
100 L=L+NBAR(K)-1
L=L+NCAV+1
IF(L.GT.KM) GO TO 40
RETURN
SUBROUTINE TRANS
INX(L,1)=NSTRT
INX(L,2)=NSTRT+8
INX(L,3)=NSTRT+NL+9
DO 4 K=4,8
4 INX(L,K)=INX(L,K-1)+NL
L=L+1
INDS(L)=NL
INDS(NSTRT)=IS
DO 11 K=2,7
11 DS(K+NSTRT-1)=TMP(K)
INDS(NSTRT+7)=KS
DS(NSTRT+NL+8)=PQ(NL+1)
DO 21 K=1,NL
DS(K+NSTRT+7)=PQ(K)
DS(K+NSTRT+NL+8)=AQ(K)
DS(K+NSTRT+2*NL+8)=AQT(K)
DS(K+NSTRT+3*NL+8)=DG(K)
INDS(K+NSTRT+4*NL+8)=ID(K)
DS(K+NSTRT+5*NL+8)=w(K)
DO 21 J=1,NL
21 DS(J+NL*K+NSTRT+5*NL+8)=FR(J+NL*K-NL)
NSTRT=NSTRT+(NL+3)**2
RETURN
END

```

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Function ERFGS collects empirical ground state excitation rates for atom or ion types k. These rates are placed in function routines and depend on the electron temperature and level index n. The functions are to return a negative value (e.g., -1.0) for levels whose rates are not calculated. The Collector replaces the dummy names EDUMYi by the functions which are associated with the replacements for LDUMYi.

Function ERFGRY is used to calculate excitation coefficients based on the classical Gryzinski cross sections (Appendix D). For nonallowed transitions, function EREG based on Gryzinski exchange cross sections is used.

-TFOR,SI SUB2

FUNCTION ERFGS(TE,N,K)

GO TO (1,2,3,4,5,6),K

C DUMMY FUNCTION REFS ARE TO BE CONVERTED BY COLLECTOR

1 ERFGS=EDUMMY1(N,TE)  
RETURN

2 ERFGS=EDUMMY2(N,TE)  
RETURN

3 ERFGS=EDUMMY3(N,TE)  
RETURN

4 ERFGS=EDUMMY4(N,TE)  
RETURN

5 ERFGS=EDUMMY5(N,TE)  
RETURN

6 ERFGS=EDUMMY6(N,TE)  
RETURN  
END

```

-TFOR,SI SUB3
FUNCTION ERFGRY(Y,A)
REAL Y,A
IND=0
IF(Y.LE.1.0E-3) GO TO 100
IF(Y.GE.30.0) GO TO 300
IF(Y.GE.0.1.AND.Y.LE.10.0) GO TO 200
IF(Y.GT.10.0) GO TO 50
X=ALOG10(Y)
IF(X.LE.-0.5-0.25*A.AND.X.LE.-2.0) GO TO 100
IF(X.GE. 0.5-0.25*A.AND.X.GE.-2.0) GO TO 200
IND=1
IF(A.LE.6.0) GO TO 10
IF(A.GE.10.0) GO TO 20
WS=X+0.5+0.25*A
GO TO 100
10 WS=X+2.0
GO TO 100
20 WS=X+3.0
GO TO 100
50 IND=2
WS=0.05*Y-0.5
GO TO 200
100 F=SQRT(Y)*(1.0-A*ALOG(A*Y)/3.0)
IF(F.LT.0.0) F=0.0
IF(IND.EQ.0) GO TO 500
FT=F
200 T=(A+30.0)/(10.0*A+25.0)
F=A**0.25*(1.143*Y*Y+2.0*Y+0.127)
F=Y**T/F
IF(IND.EQ.0) GO TO 500
IF(IND.EQ.2) GO TO 250
210 F=WS*(F-FT)+FT
GO TO 500
250 FT=F
300 T=1.5-1.0/(A+1.0)
F=1.5*SQRT(A)*Y**T
F=1.0/F
IF(IND.EQ.0) GO TO 500
GO TO 210
500 ERFGRY= 0.875*F*EXP(-Y)
RETURN
END

```

-TFOR,SI SUB4

FUNCTION EREG(Y,A,B)

X=A/100.0

IF(Y.GT.29.0) GO TO 10

C=0.8665+(4.634-2.834\*Y)\*Y\*EXP(-3.0\*Y)+1.288\*Y\*\*3\*EXP(-Y)

G=5.97\*EXP(-Y)-10.65\*EXP(-2.0\*Y)+7.85\*EXP(-3.0\*Y)

GO TO 20

10 C=0.8665

G=0.0

20 X=0.524/X-2.195+2.493\*X-0.397\*X\*X

W=2.0\*C+2.0E-2\*G\*X

X=B/10.0

FX=X-0.1

FX=6.5\*FX+10.0\*FX\*FX

IF(FX.GT.88.0) FX=88.0

C=(252.26+3.713/X+0.0307/X\*\*2)\*(1.0-EXP(-FX))

IF(X.GT.3.1) GO TO 30

G=4.0+0.0541\*X+0.247\*X\*X\*EXP(-4.0\*X\*X)+184.0\*X\*\*4\*EXP(-9.0\*X\*X)

GO TO 40

30 G=4.0+0.0541\*X

40 FX=2.013+0.2098\*X-0.0802\*X\*X

G=G\*(Y-1.0)

IF(G.GT.88.0) G=88.0

EREG=2.0E-3\* C\*Y\*\*FX\*EXP(-G)/A\*\*W

RETURN

END

Subroutine NWTH calculates the line width per unit perturber number density for atom perturbers. The perturber type index is KP and the radiator index is KR, NL denotes the number of radiator levels calculated. If the perturber is an ion, the subroutine sets logical constant TEST to true and returns. The width of the transition between lower level  $i$  and upper level  $j$  is placed in the vector W residing in TEMPS common. The storage is arranged in terms of a half-matrix (null below the diagonal). Subroutine EWTH performs a similar calculation for electron perturbers. The basic broadening theory is outlined in Appendix A. The results of these subroutines along with natural, power and rate broadening are combined in LINWID. Power and rate quenching frequencies are obtained from INCR common. The total homogeneous broadening W and Doppler broadening WD reside in TEMPS.

Subroutine CRATE calculates the collisional rate coefficient matrix  $K_{ij}$  for type KR. The matrix resides in TEMPS as the symbol RM. It is assumed that the equivalent number of ground state electrons (ANG) is contained in empirical excitation rates. Ionization rates are the matrix elements with  $j = NPL$ .

```

-TFOR,SI SUB5
  SUBROUTINE NWTH(T,KR,KP,NL,TEST,
  INCLUDE SPEC1,LIST
  PARAMETER NHSQ=(NLM+NSQ)/2
  DIMENSION W(NHSQ)
  EQUIVALENCE (IS,TMP(1)),(L,TMP(2)),(AMR,TMP(3)),(AMP,TMP(4)),
C   (ALPH,TMP(5)),(RM,TMP(6)),(K,TMP(7)),(C6,TMP(8)),(C6P,TMP(9)),
C   (C3,TMP(10)),(C3P,TMP(11)),(CU,TMP(12)),(CUP,TMP(13)),
C   (W(1),TMP(21))
  LOGICAL TEST
  F(X)=X*(X+1.0)/(7.5*X*(X+1.0)-5.625)
  TEST=.FALSE.
  K=INX(KR,1)
  IZR=INDS(K)
  J=INX(KP,1)
  L=INDS(J)
  IF(L.NE.1) GO TO 70
  IS=0
  IF(KR.EQ.1) GO TO 6
  L=KR-1
  DO 4 I=1,L
4   IS=IS+4*INDS(I+1)
6   L=INDS(KR+1)
  AMR=DS(K+1)
  IF(KR.EQ.KP) GO TO 40
  AMP=DS(J+1)
  ALPH=DS(J+4)
  RM=1.0/AMR+1.0/AMP
  RM=(T*RM)**0.3
  LS=INX(KR,4)-1
  CU=(IZR-1)
  DO 30 I=1,NL
  K=((I-1)*(2*L-I))/2
  C6=BP(I+IS+L)
  IF(IZR.EQ.1) GO TO 16
  C3=DS(I+LS)
  C3=F(C3)
  C6=C6*CU*SQRT(C3)
16  DO 30 J=I,NL
  IF(J.EQ.1) GO TO 20
  C6P=BP(J+IS+L)
  IF(IZR.EQ.1) GO TO 18
  C3=DS(J+LS)
  C3=F(C3)
  C6P=C6P*CU*SQRT(C3)
18  C6P=ALPH*ABS(C6-C6P)
  W(J+K)=1.9E-3*C6P**0.4*RM
  GO TO 30
20  W(J+K)=0.0
30  CONTINUE
  GO TO 100
40  RM=SQRT(2.0*T/AMR)
  DO 60 I=1,NL
  K=((I-1)*(2*L-I))/2
  C3=BP(I+IS)
  CU=BP(I+IS+L)
  DO 60 J=I,NL
  IF(J.EQ.1) GO TO 50
  C3P=C3+BP(J+IS)

```



```
CUP=CU+BP(J+IS+L)
C3P=0.0969*C3P
* CUP=2.04E-4*CUP*RM
W(J+K)=AMAX1(C3P,CUP)
GO TO 60
50 W(J+K)=0.0
60 CONTINUE
GO TO 100
70 TEST=.TRUE.
100 RETURN
END
```

TFOR,SI SUB6 --- 77-11

SUBROUTINE EWTH(TE,KR,NL)

INCLUDE SPEC1,LIST

PARAMETER NHSQ=(NLM+NSQ)/2

DIMENSION W(NHSQ)

EQUIVALENCE (IS,TMP(1)),(L,TMP(2)),(L1,TMP(3)),(L2,TMP(4)),(L3,  
C TMP(5)),(Z,TMP(6)),(CS,TMP(7)),(RS,TMP(8)),(KS,TMP(9)),(S,  
C TMP(10)),(TD,TMP(11)),(TR,TMP(12)),(K,TMP(13)),(C1,TMP(14)),  
C (C2,TMP(15)),(C3,TMP(16)),(C4,TMP(17)),(C1P,TMP(18)),(C3P,  
C TMP(19)),(C4P,TMP(20)),(W(1),TMP(21))

DATA A1,A2,A3,A4/0.029,12.2,5.625,7.5/

IS=0

IF(KR.EQ.1) GO TO 6

L=KR-1

DO 4 I=1,L

4 IS=IS+4\*INDS(I+1)

6 L=INDS(KR+1)

IS=IS+L

L1=INX(KR,1)

L2=INX(KR,4)-1

L3=INX(KR,6)-1

Z=INDS(L1)-1

Z=Z\*Z

CS=DS(L1+5)

RS=DS(L1+6)

KS=INDS(L1+7)

S=RS+0.5

TD=TE\*\*S

TR=SQRT(TE)

S=S/(1.0+S)

RS=TE\*\*RS

DO 50 I=1,NL

K=((I-1)\*(2\*L-I))/2

C3=DS(I+L2)

C3=C3\*(C3+1.0)

C3=C3/(C3\*A4-A3)

C3=SQRT(C3)\*BP(I+IS)

C4=BP(I+IS+L)

IF(INDS(I+L3).GT.0.OR.I.EQ.1) GO TO 10

C1=CS\*DS(I+L1+7)\*\*KS

C2=A2\*(A1\*Z/C1)\*\*S/TD

C1=RS\*C1\*AMAX1(1.0,C2)

GO TO 12

10 C1=0.0

12 CONTINUE

DO 50 J=I,NL

IF(J.EQ.I) GO TO 40

C3P=DS(J+L2)

C3P=C3P\*(C3P+1.0)

C3P=C3P/(C3P\*A4-A3)

C3P=SQRT(C3P)\*BP(J+IS)

C3P=ABS(C3-C3P)

C4P=ABS(C4-BP(J+IS+L))

IF(INDS(J+L3).GT.0.OR.J.EQ.1) GO TO 20

C1P=CS\*DS(J+L1+7)\*\*KS

C2=A2\*(A1\*Z/C1P)\*\*S/TD

C1P=RS\*C1P\*AMAX1(1.0,C2)

GO TO 22

20 C1P=0.0

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----- 77-11
22  CONTINUE
    C1P=C1+C1P
    C2=CBRT(TR*C4P*C4P)
-----
    C4P=11.14*(Z*C4P)**0.4/TR
    C4P=0.0362*AMAX1(C4P,C2)
    C4P=AMAX1(C4P,C1P)
-----
    C2=8.18*CBRT(Z*C3P*C3P)/TR
    C3P=0.0969*AMAX1(C3P,C2)
    W(J+K)=AMAX1(C3P,C4P)
-----
    GO TO 50
40  W(J+K)=0.0
50  CONTINUE
    RETURN
    END
```

```

-----
-TFOR,SI SUB7
SUBROUTINE LINWID(TE,T,ANE,AN,KR,NL)
INCLUDE SPEC1,LIST
INCLUDE SPEC4,LIST
LOGICAL TEST
IS=0
IR=0
IF(KR.EQ.1) GO TO 6
L=KR-1
DO 4 I=1,L
IS=IS+4*INDS(I+1)
4 IR=IR+INDS(I+1)
6 L=INDS(KR+1)
IS=IS+3*L
CALL EWTH(TE,KR,NL)
DO 20 I=1,NL
K=IFN(I,L)
DO 20 J=I,NL
20 W(J+K)=ANE*WD(J+K)
DO 30 K=1,NSP
CALL NWTH(T,KR,K,NL,TEST)
IF(TEST) GO TO 30
DO 25 I=1,NL
N=IFN(I,L)
DO 25 J=I,NL
W(J+N)=W(J+N)+AN(K)*WD(J+N)
25 CONTINUE
30 CONTINUE
N=INX(KR,2)-1
A=INDS(N-7)**2
A=1.415E3*SQRT(T/DS(N-6))*A
DO 50 I=1,NL
K=IFN(I,L)
B=BP(I+IS)+R(I+IR)
C=1.0/DS(I+N)**2
DO 50 J=I,NL
W(J+K)=W(J+K)+B+BP(J+IS)+R(J+IR)
50 WD(J+K)=A*(C-1.0/DS(J+N)**2)
RETURN
END
-----

```

```

SUBROUTINE CRATE(TE,KR,NL)
INCLUDE SPEC1,LIST
PARAMETER N2=NSQ+NLM+1
DIMENSION RM(NLM,NPL),STP(15)
EQUIVALENCE (RM(1,1),TMP(1)),(STP(1),TMP(N2)),(L,STP(1)),(L1,
C STP(2)),(L2,STP(3)),(L3,STP(4)),(L4,STP(5)),(ANG,STP(6)),
C (U,STP(7)),(V,STP(8)),(VP,STP(9)),(GL,STP(10)),(GU,STP(11)),
C (A,STP(12)),(B,STP(13)),(Y,STP(14)),(R,STP(15))
DATA PC/15.79/
L=INDS(KR+1)
L1=INX(KR,2)-1
L2=INX(KR,5)-1
L3=INX(KR,6)-1
L4=INX(KR,8)-L-1
ANG=INDS(L3+1)
Z=INDS(L1-7)**2
DO 60 I=1,NL
U= Z/DS(I+L1)**2
GL=DS(I+L2)
DO 50 J=I,NL
IF(J.EQ.I) GO TO 40
V=VP
VP= Z/DS(J+L1+1)**2
GU=DS(J+L2)
A=U-V
Y=A*PC/TE
R=GU*EXP(-Y)/GL
IF(I.EQ.1.AND.IABS(INDS(J+L3)).EQ.2) GO TO 30
6 B=DS(I+L*J+L4)
IF(B.LE.0.0) GO TO 20
B=A*SQRT(A)
A=U/A
RM(I,J)=ERFGRY(Y,A)/B
A=U-VP
Y=A*PC/TE
B=A*SQRT(A)
A=U/A
RM(I,J)=RM(I,J)-ERFGRY(Y,A)/B
10 IF(I.EQ.1) RM(I,J)=ANG*RM(I,J)
12 RM(J,I)=RM(I,J)/R
GO TO 50
20 B=(U-VP)/A
A=U/A
RM(I,J)=(A/U)*SQRT(A/U)*EREG(Y,A,B)
GO TO 10
30 B=ERFGS(TE,J,KR)
IF(B.LT.0.0) GO TO 6
RM(I,J)=B
GO TO 12
40 RM(I,J)=0.0
VP= Z/DS(J+L1+1)**2
50 CONTINUE
V= Z/DS(NL+L1+1)**2
A=U-V
Y=A*PC/TE
B=A*SQRT(A)
A=U/A
RM(I,NPL)=ERFGRY(Y,A)/B

```

```
IF(I.EQ.1) GO TO 54
GO TO 60
54 VP=ERFGS(TE,L+1,KR)
IF(VP.GT.C.C) GO TO 56
RM(I,NPL)=ANG*RM(I,NPL)
GO TO 60
56 Y=U*PC/TE
B=U*SQRT(U)
RM(I,NPL)=ANG*(RM(I,NPL)-ERFGRY.(Y,1.C)/B)+VP
60 CONTINUE
RETURN
END
```

Functions TVEF and AXEF give transverse or side and axial or end escape factors for inverted transitions, respectively. Least square curve fits to numerical calculations are used (see Appendix B). The arguments are C - axial gain logarithm, R - cavity aspect ratio and P - ratio of Lorentz to Doppler line widths. To avoid possible overflow problems, values of gain are limited to certain bounds in the functions. The function CSA produces the average side solid angle fraction for  $L \leq 0$ , the average end solid angle fraction for  $L = 1$ ,  $\langle r/L \rangle_{\text{side}}$  for  $L = 2$  and  $\langle r/L \rangle_{\text{end}}$  for  $L \geq 3$ . Function LPI gives  $\langle \bar{p} \rangle$  and WLP gives the line profile constant k for the input of the line width ratio.

The subroutine ESCAPE calculates the emission factors  $E_{ji}$  for the transition  $j \rightarrow i$ . (Cavity effects are not involved.) The factors use the symbol PHI and reside in TEMPS. Required input is the excited level populations ANX for type KR. The optical depth or gain logarithm is denoted by G. An expression needed for the Jacobian matrix, the rate of change of the logarithm of the emission factor with respect to the logarithm of G, is placed as the symbol W in TEMPS. If the magnitude of the excess emission (Appendix B) is less than  $10^{-3}$ , this expression equals the excess emission and is not needed; W then contains a multiplicative factor that describes the power broadening. The broadening is simply this power factor times the Einstein A-value (noncavity effects only). For the larger magnitude excess emission, the power factor equals the excess emission factor times the upper level population density and divided by the inversion density. (For absorbing transitions, both the excess emission and inversion density are negative giving a positive power factor.) Note that the excess emission and inversion density approach zero at the same rate so that the power factor as contained in W can be determined from an expression that is a limit ratio. Arrays GP and LU in TEMPS are used to store data on inverted levels in the following manner: GP(1,i) are the positive gain logarithms in order of descending values (up to i=4), GP(2,i) are the corresponding line width ratios, GP(3,i) the transition center profile values, LU(1,i) the lower level indices and LU(2,i) the upper level indices. The data corresponding to a cavity transition are used in the cavity rate equations. If a cavity transition is not one of the four maximum of gains greater than unity for a given atom or ion type, then data are not made available for the cavity and coupling of the cavity intensity to the laser medium is neglected. (The diagonal elements of the

emission factor are used to hold the total gain of a level for transitions to all lower levels. An upper bound on any neglected cavity coupling thus may be established.)



```

FOR,SI SUB9
  FUNCTION TVEF(C,R,P)
  DIMENSION A(7,3),B(3)
  DATA A/0.96213,-1.3732,4.3505,-4.7683,2.4813,-0.59608,0.052728,
C      3.1943,-7.6577,12.775,-12.875,6.6044,-1.5975,0.14369,3.8401,
C      3.7817,-15.395,17.138,-8.7419,2.0886,-0.18833/
  INCLUDE SPEC1,LIST
  INCLUDE SPEC2,LIST
  REAL LPI
  X=AMINI(3.912,ALOG(R))
  DO 10 I=1,3
  B(I)=0.0
  DO 10 J=7,1,-1
  B(I)=X*B(I)
10  B(I)=B(I)+A(J,I)
  D=CFST(3)
  ENTRY TV2(C,R,P)
  CE=C
  IF(C.GT.50.0) CE=50.0+30.0*(C-50.0)/(C-20.0)
  W=1.0/(1.0+12.5*(CE/R)**4)
  TVEF=(1.0-W)*WLP(P)*TVQ(CE)+W*CE*D*LPI(P)
  RETURN
  FUNCTION TVQ(DUM)
  X=C.1*DUM
  X=-B(1)+B(2)*X+B(3)*X*X
  IF(X.GT.10.0) X=10.0
  TVQ=EXP(X)
  RETURN
  END

```

-TFOR,SI SUB10

```

FUNCTION AXEF(C,R,P)
  DIMENSION A(6,3),B(2),CA(3)
  DATA A/-8.47794E-3,1.20125E-1,5.06073E-3,-6.86903E-3,8.67579E-4,
C      -3.25246E-5,-1.59631E-1,2.80494E-1,-1.21696E-1,2.19665E-2,
C      -1.79975E-3,5.5E-5,-1.42061E-2,1.06835E-1,-4.34725E-2,
C      6.91377E-3,-4.9476E-4,1.33524E-5/B/0.0337633,-0.0080375/
  INCLUDE SPEC1,LIST
  INCLUDE SPEC2,LIST
  REAL LPI
  CE=C
  IF(C.GT.50.0) CE=50.0+30.0*(C-50.0)/(C-20.0)
  DO 10 I=1,3
    CA(I)=0.0
  DO 10 J=6,1,-1
    CA(I)=CE*CA(I)
10  CA(I)=CA(I)+A(J,I)
    IF(CE.LE.4.0) GO TO 20
    G=B(1)+B(2)*CE
    IF(CE.GE.6.0) GO TO 19
    W=2.0**CE/16.0
    CA(2)=CA(2)+(1.0-W)*(CA(2)-G)/3.0
    GO TO 20
19  CA(2)=G
20  G=ALOG(R)
    IF(CE.LE.1.0) GO TO 40
    W=(CA(1)+CA(2)*G+CA(3)*G*G)/(CE*CE)
30  G=W*EXP(CE)*SQRT(CE)/(R*R)
    GO TO 50
40  W=0.110674+0.019389*G+0.055589*G*G
    GO TO 30
50  W=1.0/(1.0+50.0*CE)
    AXEF=(1.0-W)*G*WLP(P)+W*CE*CFST(4)*LPI(P)
  RETURN
  END

```

```

-TFOR,SI SUB11
  FUNCTION CSA(R,L)
  DIMENSION A(4,2)
  DATA A/0.4244,-0.172,0.09,-0.025,0.66,-1.09,2.3,-1.6/
  IF(L.GE.3) GO TO 30
  M=MAX0(1,L)
  B=0.0
  DO 10 I=4,1,-1
10  B=(B+A(I,M))/R
  IF(L.GT.0) GO TO 20
  CSA=1.0-B
  RETURN
20  CSA=B
  RETURN
30  CSA=(0.9428+ALOG(R))/(8.0*R*R)+0.0132/R**4
  RETURN
END
-FOR,IS SUB11B
  FUNCTION LPI(X)
  REAL LPI
  LPI=(0.707+1.25*X)/(1.0+2.5*X)
  RETURN
  END
-FOR,IN SUB11C
  FUNCTION WLP(X)
  WLP=(1.0+0.7304*X+0.5811*X*X)/(1.0+1.2946*X+1.0299*X*X)
  RETURN
  END

```

-TFOR,SI SUB12

```

SUBROUTINE ESCAPE(ANX,KR,NL,AN)
  INCLUDE SPEC1,LIST
  INCLUDE SPEC2,LIST
  INCLUDE SPEC4,LIST
  DIMENSION ANX(NLM)
  REAL LPI
  F(X)=(1.0+0.93644*X+0.3299*X*X)/(1.0+2.06482*X+1.65979*X*X+
  C 0.58473*X*X*X)
  DEP(X)=(SIGN(0.25,X)-0.75)
  L=INDS(KR+1)
  RL=L
  RL=RL+0.5
  L1=INX(KR,5)-1
  L2=INX(KR,8)-1-L
  KD=(L*(L+1))/2
  DO 10 K=1,4
  GP(1,K)=0.0
  GP(2,K)=0.0
  GP(3,K)=0.0
  LU(1,K)=0
10  LU(2,K)=0
  DO 100 K=KD,1,-1
  P=2*K
  P=RL*RL-P
  I=RL+1.0-0.5*(SQRT(P)+SQRT(P+2.0))
  J=K-IFN(I,L)
  IF(J.GT.NL.OR.J.EQ.I) GO TO 90
  P=DS(J+L1)/DS(I+L1)
  RS=1.49736E5*ABS(DS(J+L*I+L2))*CL/WD(K)
  G=RS*(ANX(J)-P*ANX(I))
  P=W(K)/WD(K)
  PF=F(P)
  IF(G.GE.0.0) GO TO 50
  PA=-G/(2.0*CAR)
  PF=PF*LPI(P)*(CFST(3)+CFST(4))
  IF((-G*PF).LT.1.0E-3) GO TO 20
  G=-G*PF
  PHI(K)=0.84*SQRT(P/PA)
  PA=0.9/(PA*SQRT(ALOG(AMAX1(PA,2.72))))
  IF(PA.GT.PHI(K)) PHI(K)=-PA
  RS=ABS(PHI(K))
  PA=5.0*RS
C  ARRAY W IS USED IN JACOBIAN MATRIX
  W(K)=(1.0+PA-PA*PA)*EXP(-PA)*RS*DEP(PHI(K))-G*EXP(-G)
  PA=RS*(1.0+PA)*EXP(-PA)+EXP(-G)
  W(K)=W(K)/PA
  PHI(K)=PA
  GO TO 30
20  PHI(K)=1.0+G*PF
  W(K)=RS*PF*ANX(J)
  GO TO 100
30  IF(ABS(PHI(K)-1.0).LT.1.0E-3) PHI(K)=1.0+SIGN(1.0E-3,PHI(K)-1.0)
  GO TO 100
50  G=G*PF
  RS=RS*PF
  DO 60 J1=1,4
  IF(G.LE.GP(1,J1)) GO TO 60
  DO 54 J2=4,1,-1

```

```

IF(J2.EQ.J1) GO TO 56
GP(1,J2)=GP(1,J2-1)
GP(2,J2)=GP(2,J2-1)
GP(3,J2)=GP(3,J2-1)
LU(1,J2)=LU(1,J2-1)
LU(2,J2)=LU(2,J2-1)
54 CONTINUE
56 GP(1,J1)=G
GP(2,J1)=P
GP(3,J1)=0.5642*PF/WD(K)
LU(1,J1)=I
LU(2,J1)=J
GO TO 62
60 CONTINUE
62 J2=1
DO 70 J1=1,NCAV
IF(ICAV(1,J1).NE.KR) GO TO 70
IF(ICAV(2,J1).NE.I) GO TO 70
IF(ICAV(3,J1).NE.J) GO TO 70
J2=0
70 CONTINUE
PA=CFST(3)
IF(J2.GT.0) PA=PA+CFST(4)
PF= PA*LPI(P)
IF((G*PF).LT.1.0E-3) GO TO 20
PHI(K)=TV2(G,CAR,P)
IF(J2.LE.0) GO TO 80
PHI(K)=PHI(K)+AXEF(G,CAR,P)
RS=TV2(1.01*G,CAR,P)+AXEF(1.01*G,CAR,P)
GO TO 85
80 RS=TV2(1.01*G,CAR,P)
85 PA=PHI(K)
PHI(K)=1.0+PA
W(K)=100.0*PA*ALOG(RS/PA)/PHI(K)
J1=J+IFN(J,L)
RS=AMIN1(G,88.0)
PHI(J1)=PHI(J1)+EXP(RS)
GO TO 30
90 PHI(K)=0.0
100 CONTINUE
RETURN
END

```

The subroutine EQUIL is used to establish an equilibrium initial excited level distribution. Let

$$\sigma^{s,z} = \sum_n \beta_n^{s,z} ,$$

then the total population of type  $s,z$  is  $N_e \sigma^{s,z} N_1^{s,z+1}$ .

If

$$p^{s,z_s} = 1 ,$$

$$p^{s,z} = \prod_{y=z+1}^{z_s} \beta_1^{s,y} ,$$

then

$$N_1^{s,z+1} = (N_e)^{z_s - z} p^{s,z} N_1^s ,$$

Specie conservation is given by  $N_s = N_1^s Q_s$  where

$$Q_s = 1 + \sum_z (N_e)^{z_s - z + 1} \sigma^{s,z} p^{s,z} .$$

Charge conservation is

$$\sum_s z_s N_s = N_e \left( 1 + \sum_s N_s \frac{\partial \ln Q_s}{\partial N_e} \right) .$$

Function  $Q_s$  is a polynomial in  $N_e$ . An initial estimate of  $N_e$  is obtained by computing the next stage ionization fraction of each type ordered with increasing  $\beta_1$ . A fraction  $\geq 0.86$  is considered equivalent to unity; when the fraction is less, the calculations are halted. The  $N_e$  estimate is used to calculate  $\partial \ln Q_s / \partial \ln N_e$  and hence a new  $N_e$ , the new and old estimate are averaged and used

to calculate a new  $N_e$ , etc., until convergence is obtained. Once  $N_e$  is known, populations are readily calculated. The symbol ANG is used for ground state populations in the subroutine rather than AN. STOR, AN and ISZ are scratch variables used for ordering; other vector quantities are self explanatory or conventional.

The subroutine QSTAT is used to establish a quasistationary initial distribution. The form of this distribution is  $N_n^{s,z} \neq 0$  if and only if  $z = z_1(s)$  and  $z = z_1 + 1, n = 1$ . That is, only one ionization stage of each specie is considered in detail. If

$$N_1^{s, z_1+1} \equiv \alpha_s N_s,$$

then

$$(1 - \alpha_s)N_s = \sum_n N_n^{s, z_1}$$

and

$$N_e = \sum_s (z_1 - 1 + \alpha_s)N_s.$$

Inputs through namelist NAME14 are  $z_1$  as IZ and P to determine  $\alpha_s$ . If P is negative,  $0 < |P| \leq 1$ , then  $\alpha_s$  is set equal to  $|P|$  for all s. If P is positive,

$$\alpha_s = \left(1 + P N_e \beta_1^{s, z_1}\right)^{-1}.$$

$P=1$  corresponds to equilibrium and  $P<1$  for a recombining plasma. Levels for  $n > 2$  are assumed quasistationary. For positive P,  $N_e$  must be obtained by an iterative procedure. If  $z_1 > z_s$  or  $z_1 \leq 0$ , then specie s is considered fully ionized into the  $z_s+1$  ground level. Populations are determined by iteration

using subroutine SRJM and starting with essentially null quasistationary levels (value of  $10^{-8}$ ). Iteration is halted when the change of ground level populations of  $z_1$  are sufficiently small.

EQUIL and QSTAT place ground state populations (AN or ANG and ANP) into MSTOR common for use by the program at integration start.



```

SUBROUTINE EQUIL
  INCLUDE SPEC1,LIST
  INCLUDE SPEC2,LIST
  INCLUDE SPEC7,LIST
  PARAMETER N13S0=1+2*(NSP+NCM)
  PARAMETER NIT=10,N13S1=NSP+14,N13S2=N13S1+NSP,N13S3=N13S2+NSP,
C   N13S4=N13S3+NSP,N13S5=N13S4+NSP
  DIMENSION BETA(NSP),SIGMA(NSP),P(NSP),AN(NSP),ISZ(NSP),STOR(NSP)
C   ANG(NSP),ANP(NCM)
  EQUIVALENCE (ANR(1),STRMTX(1)),(ANPH(1),STRMTX(1)),(ANG(1),
C   STRMTX(1)),(ANP(1),STRMTX(N13S0))
  EQUIVALENCE (L,TMP(1)),(LN,TMP(2)),(LG,TMP(3)),(MC,TMP(4)),
C   (A,TMP(5)),(B,TMP(6)),(C,TMP(7)),(D,TMP(8)),(E,TMP(9)),
C   (RI,TMP(10)),(GNS,TMP(11)),(Q,TMP(12)),(S,TMP(13)),
C   (BETA(1),TMP(14)),(SIGMA(1),TMP(N13S1)),(P(1),TMP(N13S2)),
C   (AN(1),TMP(N13S3)),(ISZ(1),TMP(N13S4)),(STOR(1),
C   TMP(N13S5)),(CGME,TMP(1)),(DGME,TMP(2)),(GLTE,TMP(3))
4  FORMAT(1H0,2X30HSUM ON Z IN SUBR EQUIL - ERROR)
5  FORMAT(1H0,2X16HSLOPE FUNCTION =1PE10.3,2X10HREL ERROR=1PE10.3,
C   2X12,1X13HSTEP IN EQUIL)
6  FORMAT(1H0,2X9HFINAL NE=1PE10.3,2X6HERROR=1PE10.3)
  DATA ERROR/1.0E-3/
  B=2.0708E-7/(TE*SQRT(TE))
  C=15.79/TE
  DO 10 K=1,NSP
  LN=INX(K,2)-1
  LG=INX(K,5)-1
  L=INX(K,1)
  GNS=DS(L+2)
  L=INDS(L)
  RI=L
  L=INDS(K+1)
  SIGMA(K)=0.0
  DO 10 J=1,L
  A=RI/DS(J+LN)
  A=B*DS(J+LG)*EXP(C*A*A)/GNS
  IF(J.NE.1) GO TO 8
  BETA(K)=A
8  SIGMA(K)=SIGMA(K)+A
10  CONTINUE
  IF(NSP.EQ.1) GO TO 17
  LN=1
  MC=1
  DO 16 K=2,NSP
  L=INX(K,1)
  L=INDS(L)
  IF(L.EQ.1) GO TO 12
  GO TO 15
12  RI=1.0
  DO 14 J=MC,LN,-1
  P(J)=RI
14  RI=RI*BETA(J)
  LN=K
15  MC=MC+1
  IF(MC.EQ.NSP) GO TO 12
16  CONTINUE
  GO TO 18
17  P(1)=1.0

```

REPRODUCIBILITY OF THIS ORIGINAL PAGE IS POOR.

```

18  ISZ(1)=1
    AN(1)=ANC(1)
    STOR(1)=BETA(1)
    IF(NSP.EQ.1) GO TO 26
    MC=1
    DO 24 K=2,NSP
    L=INX(K,1)
    L=INDS(L)
    IF(L.EQ.1) MC=MC+1
    RI=ANC(MC)
    AN(K)=RI
    STOR(K)=BETA(K)
    ISZ(K)=K
    DO 20 J=K,2,-1
    IF(BETA(K).GT.STOR(J-1)) GO TO 24
    ISZ(J)=ISZ(J-1)
    ISZ(J-1)=K
    AN(J)=AN(J-1)
    AN(J-1)=RI
    STOR(J)=STOR(J-1)
    STOR(J-1)=BETA(K)
20  CONTINUE
24  CONTINUE
26  GNS=0.0
    DO 40 J=1,NSP
    RI=AN(J)*STOR(J)
    B=GNS*STOR(J)+1.0
    D=4.0*RI/(B*B)+1.0
    IF(B.LT.1.09.AND.D.LT.1.30) GO TO 36
    A= B*(SQRT(D)-1.0)/(2.0*RI)
    ANE=A*AN(J)+GNS
    GO TO 42
36  GNS=GNS+AN(J)
40  CONTINUE
42  NSTP=1
44  C=0.0
    D=1.0
    LN=1
    DO 60 J=1,NC
    GNS=ANC(J)
    IF(J.EQ.NC) GO TO 48
    LG=IC(J+1)-1
    GO TO 50
48  LG=NSP
50  L=INX(LG,1)
    L=INDS(L)
    RI=L
    C=C+RI*GNS
    MC=0
    RI=0.0
    Q=1.0
    DO 54 K=LN,LG,1
    MC=MC+1
    B=SIGMA(K)*P(K)*ANE**(L-MC)
    Q=Q+ANE*B
    A=L-MC+1
54  RI=RI+A*B
    D=D+RI*GNS/Q
    IF(LG.EQ.NSP) GO TO 62

```

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```

LN=LG+1
IF(L.NE.MC) WRITE(6,4)
60 CONTINUE
62 GNS=C/D
E=(GNS-ANE)/GNS
IF(NSTP.EQ.1) GO TO 64
IF(ABS(E).LT.1.0E-8) GO TO 64
S=D+2.0*(D-S)/E
IF(NSTP.GE.NIT.OR.S.LE.0.0) WRITE(6,5) S,E,NSTP
64 S=D
ANE=0.5*(GNS+ANE)
IF(ABS(E).LT.ERROR.OR.NSTP.GE.NIT) GO TO 70
NSTP=NSTP+1
GO TO 44
70 LN=1
IF(NSTP.LT.NIT) GO TO 71
IF(ABS(E).LT.0.01) GO TO 71
NSTP=NSTP+1
IF(NSTP.LT.3*NIT) GO TO 44
WRITE(6,6) ANE,E
71 CONTINUE
DO 80 J=1,NC
GNS=ANC(J)
IF(J.EQ.NC) GO TO 72
LG=IC(J+1)-1
GO TO 74
72 LG=NSP
74 L=INX(LG,1)
L=INDS(L)
MC=0
Q=1.0
DO 76 K=LN,LG,1
MC=MC+1
76 Q=Q+SIGMA(K)*P(K)*ANE**(L-MC+1)
MC=0
DO 78 K=LN,LG,1
MC=MC+1
78 BETA(K)=GNS*P(K)*ANE**(L-MC)/Q
IF(LG.EQ.NSP) GO TO 82
LN=LG+1
80 CONTINUE
82 MC=0
DO 90 K=1,NSP
L=INDS(K+1)
GNS=BETA(K)
DO 90 J=1,L
MC=MC+1
90 ANB(MC)=GNS
CALL CONSRV(GT,ANP,G1,G2,G3,G4,ANG,0)
E=(ANE-GT)/GT
ANE=GT
WRITE(6,6) ANE,E
CGME=0.0
DGME=0.0
CALL ELEN(GT,0.0,0.0,0.0,ANG,ANP)
GLTE=GT
RETURN
END

```

```

SUBROUTINE QSTAT
INCLUDE SPEC1,LIST
INCLUDE SPEC2,LIST
INCLUDE SPEC7,LIST
DIMENSION NBR5(NSP),ALPH(NCM),BETG(NCM),IS(NCM),KS(NCM),IZS(NCM),
C ANP(NCM),AN(NSP),R3(NLM),LC(4),D(6),R1(NLM,NPL),R2(NLM,NPL),
C R4(2,4),R5(4),R6(3,4),IZ(NCM)
LOGICAL LGP,LERR
PARAMETER N1=2*NSP+NCM+1,N2=N1+5*NCM+6,N3=N2+2*(NLM+NSQ),
C N14S1=NSP+1,N14S2=N14S1+NSP,N14S3=N1+NCM,N14S4=N14S3+NCM,
C N14S5=N14S4+NCM,N14S6=N14S5+NCM,N14S7=N14S6+NCM,N14S8=N2+NLM+
C NSQ,N14S9=N3+NLM,NIT=10
EQUIVALENCE (CGME,TMP(1)),(DGME,TMP(2)),(GLTE,TMP(3)),(AN(1),
C STRMTX(1)),(NBR5(1),STRMTX(N14S1)),(ALPH(1),STRMTX(N14S2)),
C (BETG(1),STRMTX(N1)),(ANP(1),STRMTX(N14S3)),(IZS(1),
C STRMTX(N14S4)),(IS(1),STRMTX(N14S5)),(KS(1),STRMTX(N14S6)),
C (D(1),STRMTX(N14S7)),(R1(1,1),STRMTX(N2)),(R2(1,1),
C STRMTX(N14S8)),(R3(1),STRMTX(N3)),(R4(1,1),STRMTX(N14S9)),
C (ANR(1),STRMTX(1))
NAMELIST/NAME14/ERROR,P,IZ
1 FORMAT(1H0,3X18HQSTAT ERROR, TYPE I2)
2 FORMAT(1H0,3X14HQSTAT NE DIFF=1PE10.3)
3 FORMAT(1H0,3X14HQSTAT NG DIFF=1PE10.3)
4 FORMAT(1H0,3X15HQSTAT GIVES NE=1PE10.3)
READ(5,NAME14)
LIO=0
LGP=.FALSE.
DO 10 K=1,ND
BT(K)=0.0
10 ANB(K)=1.0E-8
DO 11 K=1,NSP
AN(K)=0.0
NBR5(K)=NBAR(K)
11 NBAR(K)=2
DO 12 K=1,4
12 ANPH(K)=0.0
C=2.0708E-7/(TE*SQRT(TE))
IF(P.LT.0.0) GO TO 50
DN=0.0
A=15.79/TE
DO 20 J=1,NC
ANP(J)=0.0
IS(J)=0
KS(J)=0
K1=IC(J)
IF(J.LT.NC) K2=IC(J+1)-1
IF(J.EQ.NC) K2=NSP
MK=K2-K1+1
IF(IZ(J).GT.MK) GO TO 18
IF(IZ(J).LE.0) GO TO 19
DO 15 K=K1,K2
MK=K-K1+1
IF(MK.NE.IZ(J)) GO TO 15
Z=MK
MK=INX(K,1)+2
GD=DS(MK)
MK=INX(K,5)
GD=DS(MK)/GD

```

```

MK=INX(K,2)          77-11
Z=Z/DS(MK)
BETG(J)=C*GD*EXP(A*Z*Z)
B=IZ(J)-1
GO TO 20
15 CONTINUE
18 IZ(J)=-IZ(J)
19 BETG(J)=0.0
B=MK-1
20 DN=DN+B*ANC(J)
IT=C
ANE=DN
24 Y=0.0
DO 30 J=1,NC
30 Y=Y+ANC(J)/(1.0+P*ANE*BETG(J))
A=DN+Y
IT=IT+1
B=(ANE-A)/A
ANE=(ANE+A)/2.0
IF(ABS(B).LT.ERROR.OR.IT.GT.NIT) GO TO 32
GO TO 24
32 IF(IT.GT.NIT) GO TO 36
33 DO 34 J=1,NC
34 ALPH(J)=1.0/(1.0+P*ANE*BETG(J))
GO TO 60
36 WRITE(6,2) B
IF(ABS(B).LE.0.01) GO TO 33
IF(IT.LT.2*NIT) GO TO 24
IF(ABS(B).GT.0.05) GO TO 41
GO TO 33
40 WRITE(6,1) LIO
STOP
41 LIO=1
GO TO 40
42 LIO=2
GO TO 40
44 LIO=4
GO TO 40
45 LIO=5
GO TO 40
50 A=0.0
IF(ABS(P+0.5).GE.0.5) GO TO 42
DC 56 J=1,NC
ANP(J)=0.0
IS(J)=0
KS(J)=0
ALPH(J)=-P
IF(J.LT.NC) K2=IC(J+1)-1
IF(J.EQ.NC) K2=NSP
IT=K2+1-IC(J)
IF(IZ(J).GT.IT) IZ(J)=-IZ(J)
IF(IZ(J).GT.0) GO TO 52
B=IT
GO TO 56
52 B=IZ(J)-1
B=B-P
56 A=A+B*ANC(J)
ANE=A
60 DO 61 J=1,NC

```

```

61  ALPH(J)=ALPH(J)*ANC(J)
    MK=C
    QM=C.C
    DO 64 J=1,NC
    K1=IC(J)
    IF(J.LT.NC) K2=IC(J+1)-1
    IF(J.EQ.NC) K2=NSP
    IZS(J)=K2-K1+1
    B=IZS(J)
    QM=QM+B*ANC(J)
    DO 63 K=K1,K2
    IT=K-K1+1
    IF(IT.NE.IZ(J)) GO TO 63
    KS(J)=K
    IT=MK+1
    IS(J)=IT
    AN(K)=ANC(J)-ALPH(J)
    BT(IT)=BETG(J)
    ANB(IT)=AN(K)/(ANE*BETG(J))
    IF(K.EQ.K2) GO TO 62
    AN(K+1)=ALPH(J)
    A=15.79/TE
    Z=IZ(J)+1
    IT=INX(K+1,2)
    Z=Z/DS(IT)
    IT=INX(K+1,5)
    GD=DS(IT)
    IT=INX(K+1,1)+2
    GD=GD/DS(IT)
    B=C*GD*EXP(A*Z*Z)
    IT=IS(J)+INDS(K+1)
    BT(IT)=B
    ANB(IT)=ALPH(J)/(ANE*B)
    GO TO 63
62  ANP(J)=ALPH(J)
63  MK=MK+INDS(K+1)
64  CONTINUE
    IT=0
70  DN=0.0
    A=0.0
    B=0.0
    C=J.C
    DO 80 J=1,NC
    IF(IZ(J).LE.0) GO TO 78
    ANHS=0.0
    K=KS(J)
    MK=INDS(K+1)+IS(J)
    BTPL=BT(MK)
    IF(IZS(J).NE.IZ(J)) GO TO 71
    ANHS=ALPH(J)
    BTPL=1.0/ANE
71  MK=IS(J)-1
    ZS=IZS(J)
    Z=IZ(J)
    GD=ANB(MK+1)
    ANEP=ANE
    CALL SRJM(R1,R2,R3,AI,AR,ARR,QRI,QRR,K,MK,AN,ANEP,QM,ANPH,ANHS,
    BTPL,0.0,0.0,0.0,ZS,Z,D(1),LC,R4,LGP,J,0,D(2),D(3),D(4),D(5),
    D(6),LERR,K1,R5,R6)

```

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IF(LERR) GO TO 44
ZS=ZS+1.0-Z
A=A+ZS*(ANE*AI-ALPH(J)*AR)
B=B+ZS*ALPH(J)*ARK
C=C+ANE*(ALPH(J)*QRR-ANE*GRI)
MK=IS(J)
ANHS=0.0
K1=NSTAR(K)-2
IF(K1.LT.1) GO TO 73
DO 72 K2=1,K1
72 ANHS=ANHS+ANE*BT(MK+K2)*ANB(MK+K2)
73 ANHS=ANC(J)-ALPH(J)-ANHS
IF(ANHS.LT.0.0) ANHS=0.0
ANHS=ANHS/(ANE*BT(MK))
ZS=(GD+ANHS)/2.0
IF(ZS.EQ.0.0) GO TO 75
Z=ABS(GD-ANHS)/ZS
IF(Z.GT.DN) DN=Z
75 ANB(MK)=ZS
AN(K)=ANE*ZS*BT(MK)
78 IF(J.LT.NC) GO TO 80
IT=IT+1
IF(DN.LT.ERROR.OR.IT.GT.NIT) GO TO 82
80 CONTINUE
GO TO 70
82 IF(IT.GT.NIT) GO TO 84
GO TO 86
84 WRITE(6,3) DN
IF(DN.GT.0.05) GO TO 45
86 WRITE(6,4) ANE
DO 90 K=1,NSP
90 NBAR(K)=NBR(K)
CALL ELEN(DN,0.0,C,A,AN,ANP)
CGME=A
DGME=A+B
GLTE=DN
RETURN
END

```

Subroutine CONSRV calculates the electron density and densities of maximum ionization given the electron temperature and excited level normal populations. Densities of ground levels are also output. Symbol EPD is used for the electron density, EP is the equilibrium bound states factor  $\epsilon$ ,  $DI = 2a_0/\lambda_D$  is proportional to the lowering of the ionization potential,  $DEL = A/N_e - B$  (see conservation discussion in main text) is a measure of the correction term for finite  $\epsilon$  in  $N_e$ ,  $QM = (1 + D)N_e$  is needed by subroutine SRJM and IBT is set  $\leq 0$  if array BT of Saha factors is to be calculated and  $>0$  if not (e.g., during a second pass at a particular electron temperature).



```

-TFOR,SI SUB15
  SUBROUTINE CONSRV(EPD,ANP,EP,DI,DEL,QM,AN,IBT)
  INCLUDE SPEC1,LIST
  INCLUDE SPEC2,LIST
  PARAMETER N15S1=NCM+9,N15S2=N15S1+NCM,N15S3=N15S2+NCM,N15S4=
  C N15S3+NCM
  DIMENSION ANP(NCM),SA(NCM),SB(NCM),SC(NCM),SD(NCM),ZC(NCM),AN(NSP)
  EQUIVALENCE (MS,TMP(1)),(MR,TMP(2)),(GP,TMP(3)),(ZC,TMP(N15S4)),
  C (A,TMP(5)),(B,TMP(6)),(C,TMP(7)),(D,TMP(8)),(SA(1),TMP(9)),
  C (SB(1),TMP(N15S1)),(SC(1),TMP(N15S2)),(SD(1),TMP(N15S3))
  DO 2 J=1,NCM
    SA(J)=0.0
    SB(J)=0.0
    SC(J)=0.0
  2 SD(J)=0.0
    MS=0
    MR=0
    IF(IBT.GT.0) GO TO 3
    A=15.79/TE
    C=2.0708E-7/(TE*SQRT(TE))
  3 DO 10 K=1,NSP
    L1=INX(K,2)-1
    L2=INX(K,5)-1
    L=INX(K,1)
    GP=DS(L+2)
    L=INDS(L)
    IF(L.EQ.1) MS=MS+1
    ZC(1)=L
    L=INDS(K+1)
    DO 10 J=1,L
      MR=MR+1
      IF(J.GE.NSTAR(K)) GO TO 10
      IF(IBT.GT.0) GO TO 4
      B=ZC(1)/DS(J+L1)
      B=C*DS(J+L2)*EXP(A*B*B)/GP
      BT(MR)=B
      GO TO 6
  4 B=BT(MR)
  6 B=B*ANP(MR)
    D=ZC(1)-1.0
    SA(MS)=SA(MS)+B
    SC(MS)=SC(MS)+B*D
    IF(J.NE.1) GO TO 10
    AN(K)=B
    D=D*SQRT(D)
    SB(MS)=SB(MS)+B*D
    SD(MS)=SD(MS)+B*D*(ZC(1)-2.0)
  10 CONTINUE
    C=0.0
    D=1.0
    DO 20 J=1,NC
      IF(J.EQ.NC) GO TO 12
      K=IC(J+1)-1
      GO TO 14
  12 K=NSP
  14 L=INX(K,1)
    L=INDS(L)
    ZC(J)=L
    C=C+ZC(J)*ANP(J)

```

```

20  D=D+ZC(J)*SA(J)-SC(J)
    CONTINUE
    EPD=C/D
    EP=TE+TE*TE/T
    EP=EPD/EP**3
    EP=SQRT(EP)
    EP=1.3E-2*SQRT(EP)
    A=0.0
    B=0.0
    DO 30 J=1,NC
    GP=ZC(J)*SQRT(ZC(J))
    ANP(J)=1.0+EP*GP
    A=A+GP*ANC(J)/ANP(J)
    B=B+SD(J)-ZC(J)*SB(J)+GP*(SA(J)+EP*SB(J))/ANP(J)
30  CONTINUE
    EPD=(C-EP*A)/(D-EP*B)
    DEL=A/EPD-B
    QM=D*EPD
    DI=4.85E-4*SQRT(EPD/TE+EPD/T)
    DO 40 J=1,NC
40  ANP(J)=(ANC(J)-EPD*(SA(J)+EP*SB(J)))/ANP(J)
    DO 50 K=1,NSP
50  AN(K)=EPD*AN(K)
    RETURN
    END

```

Subroutine SRJM is used to compute rates and the Jacobian for a particular atom or ion. The argument list is as follows.

- RL rate matrix for the reduced set of equations. The vector  $G_n$  used to couple to the next ionization stage is the set of elements in RL with second index NPL.
- JCB Jacobian matrix for the reduced equations. The element set with second index NPL is the vector

$$\left( (z_s + 1 - z) N_e \right)^{-1} \left( \partial R_e / \partial \bar{N}_n \right) ,$$

used for cross terms in the overall Jacobian.

- F the vector  $\partial R_n / \partial N_e$ , plus  $(1 + D) \partial R_n / \partial N_i^+$  if  $z = z_s$ , also used for cross terms
- AI ionization coefficient
- AR recombination coefficient (collisional and radiative)
- ARR radiative recombination coefficient
- QCRI coefficient of energy absorption divided by  $kT_e$
- QCRR recombination heating coefficient divided by  $kT_e$
- KS atom or ion type index (input)
- MS location of ground level in ANB, BT vectors
- AN ground level density vector (input)
- ANEP predicted value of  $N_e$  (input)
- QM  $(1 + D) N_e$  (input, may be obtained from CONSRV)
- NPH photon density vector (input)
- ANHS  $N_1^s$  (input)
- BETAPL  $\beta_1^{z+1}$  (input)
- GLTE  $(d/dt) \ln T_e$  (input)
- CGME predicted  $R_e$  (input)
- DGME  $N_e \partial R_e / \partial N_e$  (input)
- ZS maximum specie charge number (input)
- ZC parent ion charge number (input)
- ANPL  $\bar{N}_1^{z+1}$  (output)
- IC if  $LC(j) = k > 0$ , then index k is used in the GP and LU data arrays in TEMPS common for cavity equation j

CVP cavity rate matrix: CVP(1,j) is the induced transition rate for cavity j and CVP(2,j) is the total spontaneous emission rate. The equation is

$$\frac{d}{dt} N_{ph}(j) = CVP(1,j) + \eta_e CVP(2,j) .$$

LGP logical constant set to true for consideration of the Penning effect

NCORE specie index (input)

NEXP index for excited level of Penning effect (set negative for donor)

KPEN Penning rate constant (set negative for two electron excitation)

RPEN net Penning rate (output)

ANMET metastable density at first input (to receptor atom)

ANMEQ equilibrium metastable density at first input

EMET metastable excitation energy divided by  $kT_e$  at first input

LERR logical constant output, set true in case of a matrix singularity that prevents an inversion (quasistationary levels)

IGMX location of maximum positive noncavity gain in TEMPS data arrays GP and LU. Set null if there are no inversions or if all inversions are coupled to the cavity.

FMD vector containing the mode spacing parameters  $p_0 \Delta v$

CVOUT cavity output array: CVOUT(1,j) is the gain logarithm and CVOUT(2,j) is the transition width ratio for cavity j

The function  $E_1(x)$  is used in the calculation of radiative recombination; it is approximated by the define procedure FX. At the start of the subroutine, the collisional rate coefficient matrix is placed in JCB. Values of normal density for the atom or ion are placed in ANR. Corresponding Saha factors are placed in BETA. Array AM and SRMR are used to hold derivative forms of the rate matrix with respect to populations.

The internal subroutine CAVITY calculates the cavity rate coefficient  $C = sw/t_c$  and its logarithmic derivative with respect to the gain logarithm, RCP. The internal subroutine INVERS calculates the inverse of an upper quadrant of matrix AMS (corresponding to the quasistationary level indices) and multiplies

the inverse into the array BVS composed of other elements of AMS and possibly vector F. These operations serve in the formation of reduced rate and Jacobian matrices.

The vector  $\partial N_e / \partial \bar{N}_n$  is proportional to the vector of Saha factors; it is used in calculating cross terms involving different atom or ion types. The 'reduced' form of the Saha factors is output through STORE common in symbol ANR. Also at output, GP(3,i) contains the relevant transition escape factor for  $i \geq \text{IGMX} > 0$ , and for cavity transitions contains the upper level to ground escape factor.

The Penning source code uses the following conventions. For two electron excitation, the rate constant KPEN is set negative in calls involving the receptor specie. Donor status is indicated by setting level index NEXP negative. In receptor calls, NEXP equals the total level increment and is  $\leq n^*$  for one electron excitation/ionization,  $> n^*$  for the two electron case in the receptor atom call. For the two electron case or single ionization, the receptor (single charge) ion type must also be called with the Penning effect invoked (LGP true) and with  $\text{NEXP} \leq n^*$ . Inputs to the receptor ion call are obtained from the atom call outputs. Consider the increment  $\delta F_n$  in an appropriate element of vector F due to added Penning rates. ANMET contains  $(-\beta_1 \delta F_1)$  for the atom at output. If u denotes the receptor ion terminal level ( $1 \leq u \leq n^*$ ), the receptor ion input  $\text{ANMET} = \beta_u \delta F_u$ . For ionization plus excitation, these are equal and the ANMET value is simply passed in the calls; for single or double ionization,  $\text{RPEN}/N_e^2$  must be added to ANMET between calls. Also at receptor atom output ( $\text{NEXP} \geq n^*$  at input), the equilibrium density is multiplied by  $\beta_1$  and the ionization potential is subtracted from the metastable energy. Both these new forms are passed as inputs to the ion call. The final call to SRJM involving the Penning effect is that of the donor. Inputs are: ANMET - the equilibrium donor ground level density based on the upper level density, ANMEQ - the actual ground level density, and RPEN -  $(\beta_1 \delta F_1)$  for the donor which equals the negative of the same expression for the receptor (ANMET receptor atom output). During any call invoking the Penning effect, the excitation/ionization energy is subtracted from the EMET input. After the last receptor specie call, the increment in the electron rate heating is thus the product of the output EMET and the rate RPEN.

```

-TFOR,SI SUB16
  SUBROUTINE SRJM(RL,JCB,F,AI,AR,ARR,QCRI,QCRR,KS,MS,AN,ANEP,QM,NPH,
C   ANHS,BETAPL,GLTE,CGME,DGME,ZS,ZC,ANPL,LC,CVP,LGP,NCORE,NEXP,
C   KPEN,RPEN,ANMET,ANMEQ,EMET,LERR,IGMX,FMD,CVOUT)
  INCLUDE SPEC1,LIST
  INCLUDE SPEC2,LIST
  INCLUDE SPEC4,LIST
  INCLUDE SPEC6,LIST
  REAL JCB,KPEN,NPH(4),LPI
  LOGICAL LGP,LGI,LPRNT,LGL,LERR
  PARAMETER NWS=4*NLM,NPP=NPL+1,KBV=(NPP*NPP)/4,
C   NSBT=2*NLM+1,NRF1=NPL+KBV+NLM
  DIMENSION RL(NLM,NPL),JCB(NLM,NPL),F(NLM),ANX(NLM),BETA(NLM),
C   ANR(NLM),LC(4),BVS(KBV),AM(NLM,NLM),DW(NWS),RMT(NLM,NPL),
C   CVP(2,4),FMD(4),CVOUT(3,4)
  EQUIVALENCE(SV(1),ANR(1)),(SV(NPL),BETA(1)),(SV(NSBT),BVS(1)),
C   (TMP(21),DW(1)),(SV(NRF1),AM(1,1)),(TMP(1),RMT(1,1)),
C   (SV(NSBT),ANX(1))
  FX(X)=1.12*EXP(-X)/(X+0.935*X**0.3)
  DATA S6/7.95775E-2/LPRNT/.TRUE./
111  FORMAT(1H0,3X31HIMPROPER PENNING RECEPTOR LEVEL)
112  FORMAT(4X22HPENNING EFFECT IGNORED)
113  FORMAT(1H0,4X20HRATE MATRIX SINGULAR)
114  FORMAT(1H0,4X24HJACOBIAN MATRIX SINGULAR)
  LERR=.FALSE.
  IRST=MS
  LN=INX(KS,2)-1
  LG=INX(KS,5)-1
  LW=INX(KS,7)-1
  LF=INX(KS,8)-1
  L=INX(KS,1)+2
  GNS=DS(L)
  L=INDS(KS+1)
  LF=LF-L
  NB=NBAR(KS)
  NL=NSTAR(KS)-1
  CALL CRATE(TE,KS,NL)
  DO 10 K=1,NL
  JCB(K,NPL)=RMT(K,NPL)
  DO 10 J=1,NL
  RL(J,K)=0.0
10  JCB(J,K)=RMT(J,K)
  DO 12 K=1,L
  IF(K.EQ.NB) MR=MS
  MS=MS+1
12  ANR(K)=ANB(MS)
  ANPL=ANHS
  IF(ZC.LT.ZS) ANPL=ANB(MS+1)
  S1=2.0708E-7/(GNS*TE*SQRT(TE))
  S2=15.79*ZC*ZC/TE
  S3=157.46*ZC**4*GNS
  S4=DS(NL+LN+1)**2
  S4=S2/S4
  S5=1.0
  IF(ZC.LT.ZS) S5=ANEP*BETAPL
  AI=0.0
  AR=0.0
  ARR=0.0
  QCRI=0.0

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QCRR=0.0
DO 20 K=1,NL
  RSUM=0.0
  DO 22 J=1,NL
    22 RSUM=RSUM+JCB(K,J)*(ANR(K)-ANR(J))
  C ARRAY F IS USED IN THE JACOBIAN MATRIX
    F(K)=(S5*ANPL-ANR(K))*JCB(K,NPL)-RSUM
    IF(K.LT.NB) F(K)=F(K)-ANR(K)*DGME/ANEP
    Q=DS(K+LN)**2
    U=S2/Q
    A=S3*DS(K+LW)*FX(U-S4)/(DS(K+LG)*Q*DS(K+LN))
    Q=S1*DS(K+LG)*EXP(U)
    ARR=ARR+Q*A
    ANX(K)=ANEP*Q*ANR(K)
  C ARRAY BETA IS USED IN THE JACOBIAN MATRIX
    BETA(K)=Q
    A=A+ANEP*JCB(K,NPL)
    AR=AR+Q*A
    QCRR=QCRR+Q*U*A
    A=S5*A
    RL(K,NPL)=A
    SRMR=ANPL
    IF(.NOT.(ZC.LT.ZS)) SRMR=SRMR+QM-ANC(NCORE)
    F(K)=F(K)+A*SRMR/ANEP
    A=Q*ANR(K)*JCB(K,NPL)
    AI=AI+A
    QCRI=QCRI+U*(A+Q*RSUM)
  20 CONTINUE
    CALL LINWID(TE,T,ANEP,AN,KS,NL)
    CALL ESCAPE(ANX,KS,NL,AN)
    DO 25 K=1,4
      LC(K)=0
      IF(ICAV(1,K).NE.KS) GO TO 25
      CVP(1,K)=0.0
      CVP(2,K)=0.0
      DO 24 J=1,4
        IF(ICAV(2,K).NE.LU(1,J)) GO TO 24
        IF(ICAV(3,K).NE.LU(2,J)) GO TO 24
      LC(K)=J
    24 CONTINUE
      IF(LC(K).EQ.0) LC(K)=-1
    25 CONTINUE
      S3=0.5101*S3/GNS
      DO 48 J=1,NL
        S1=0.0
        S4=0.0
        RSUM=0.0
        U=0.0
        SRMR=0.0
        R(J+IRST)=0.0
        R1=1.0/DS(J+LN)**2
        DO 46 K=1,NL
          IF(J.EQ.K) GO TO 46
          RL(J,K)=ANEP*JCB(J,K)
          S1=S1+RL(J,K)
          Q=R1-1.0/DS(K+LN)**2
          A=S3*Q*Q
          R2=DS(K+LG)/DS(J+LG)
          R3=RFTA(K)/RFTA(J)

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R4=ANR(K)/ANR(J)
IF(J.GT.K) GO TO 37
A=A*ABS(DS(K+L*J+LF))
IS=K+IFN(J,L)
Q=R3*A*PHI(IS)
RL(J,K)=RL(J,K)+Q
LGI=(ABS(PHI(IS)-1.0).LT.1.0E-3)
IF(LGI) AM(J,K)=Q*(PHI(IS)-1.0)
IF(.NOT.LGI) AM(J,K)=Q*W(IS)
RSUM=RSUM+AM(J,K)*ANR(K)
IF(.NOT.LGI) GO TO 27
AM(J,K)=Q*W(IS)
SRMR=SRMR-R2*AM(J,K)/R3
27 Q=1.0/(R3*R4)-1.0/R2
IF(LGI) GO TO 28
IF(ABS(Q).LT.1.0E-7) Q=SIGN(1.0E-7,Q)
SRMR=SRMR+AM(J,K)/(R3*Q)
AM(J,K)=-AM(J,K)/(R2*Q)
28 IF(NCAV.LE.0) GO TO 36
DO 35 J1=1,NCAV
I=LC(J1)
IF(I.LE.0) GO TO 35
IF(LU(1,I).NE.J) GO TO 35
IF(LU(2,I).NE.K) GO TO 35
CALL CAVITY(RC,RCP,GP(1,I),GP(2,I),GP(3,I),FMD(J1))
CVOUT(1,J1)=GP(1,I)
CVOUT(2,J1)=GP(2,I)
CVP(1,J1)=RC*NPH(J1)
IF((-R2*Q).LE.1.0E-6) GO TO 29
RCP=NPH(J1)*(RCP-RC)
CVP(2,J1)=RCP
RCP=RCP*R3/ANX(K)
AM(J,K)=AM(J,K)-RCP/(R2*Q)
SRMR=SRMR+RCP/(R3*Q)
RSUM=RSUM+CVP(2,J1)/(ANEP*BETA(J))
RC=R3*CVP(1,J1)/ANX(K)
S1=S1-RC/(R3*Q)
RL(J,K)=RL(J,K)-RC/(R2*Q)
GO TO 30
29 CVP(2,J1)=-1.0
30 IGMX=K+IFN(1,L)
GP(3,I)=PHI(IGMX)
35 CONTINUE
36 A=S6*A
IF(LGI) A=R2*A
GO TO 45
37 A=A*ABS(DS(J+L*K+LF))
IS=J+IFN(K,L)
Q=A*PHI(IS)
S4=S4+Q
LGI=(ABS(PHI(IS)-1.0).LT.1.0E-3)
IF(LGI) AM(J,K)=Q*(PHI(IS)-1.0)
IF(.NOT.LGI) AM(J,K)=Q*W(IS)
U=U+AM(J,K)
IF(.NOT.LGI) GO TO 38
Q=Q*W(IS)
AM(J,K)=R3*Q/R2
SRMR=SRMR-Q
38 Q=R3*R4/R2-1.0

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ST=R2/R3-R4
IF(LGI) GO TO 39
IF(ABS(Q).LT.1.0E-7) Q=SIGN(1.0E-7,Q)
IF(ABS(ST).LT.1.0E-7) ST=SIGN(1.0E-7,ST)
SRMR=SRMR+AM(J,K)/Q
AM(J,K)=AM(J,K)/ST
39 IF(NCAV.LE.0) GO TO 44
DO 42 J1=1,NCAV
I=LC(J1)
IF(I.EQ.0) GO TO 42
IF(I.LT.0) GO TO 41
IF(LU(1,I).NE.K) GO TO 42
IF(LU(2,I).NE.J) GO TO 42
IF(CVP(2,J1).LT.0.0) GO TO 40
RCP=CVP(2,J1)
RCP=RCP/ANX(J)
AM(J,K)=AM(J,K)+RCP/ST
SRMR=SRMR+RCP/Q
RSUM=RSUM-CVP(2,J1)/(ANEP*BETA(J))
RC=CVP(1,J1)/ANX(J)
S1=S1-RC/Q
RL(J,K)=RL(J,K)+RC/ST
40 CVP(1,J1)=CVP(1,J1)-NPH(J1)*FCAV
CVP(2,J1)=A*ANX(J)
GO TO 42
41 IF(ICAV(2,J1).NE.K) GO TO 42
IF(ICAV(3,J1).NE.J) GO TO 42
GO TO 40
42 CONTINUE
44 A=S6*A
45 IF(LGI) A=A*W(IS)
IF(.NOT.LGI) A=A*(1.0-PHI(IS))/Q
R(J+IRST)=R(J+IRST)+A
46 CONTINUE
S1=S1+ANEP*JCB(J,NPL)
RL(J,J)=-S1-S4
AM(J,J)=SRMR
F(J)=F(J)+(RSUM-U*ANR(J))/ANEP
R(J+IRST)=R(J+IRST)+S6*S1
IF(J.GE.NB) GO TO 48
Q=1.5+S2*R1
RL(J,J)=RL(J,J)+Q*GLTE-CGME
Q=ANEP*(ZS+1.0-ZC)*ANR(J)
DO 47 K=1,NL
47 AM(J,K)=AM(J,K)-Q*BETA(K)*JCB(K,NPL)
48 CONTINUE
C FORM JACOBIAN MATRIX
S1=ANEP*ANEP*(ZS+1.0-ZC)/QM
DO 49 J=1,NL
JCB(J,NPL)=BETA(J)*JCB(J,NPL)
DO 49 K=1,NL
49 JCB(K,J)=RL(K,J)+AM(K,J)-S1*F(K)*BETA(J)
C START PENNING SOURCE CODE
C PENNING EFFECT TEST
IF(.NOT.LGP) GO TO 90
LGI=.TRUE.
IF(NEXP.GE.NSTAR(KS)) GO TO 70
IF(KPEN.LT.0.0.OR.NEXP.EQ.1) GO TO 80
IF(NEXP.GE.NB) GO TO 60

```

```

50  IS=IABS(NEXP)
    R1=BETA(1)/BETA(IS)
    R2=ANMET*KPEN
    R3=ANMEQ*KPEN
    IF(NEXP.GT.0) GO TO 51
    R2=R2/R1
    R3=R3/R1
    NEXP=-NEXP
    R4=-RPEN/BETA(1)
    GO TO 52
51  R4=R2*ANR(1)-R3*ANR(NEXP)
    RPEN=ANEP*BETA(1)*R4
    R4=R4/ANEP
52  RL(NEXP,1)=RL(NEXP,1)+R1*R2
    JCB(NEXP,1)=JCB(NEXP,1)+R1*R2
    RL(1,NEXP)=RL(1,NEXP)+R3
    JCB(1,NEXP)=JCB(1,NEXP)+R3
53  Q=1.0/DS(1+LN)**2-1.0/DS(NEXP+LN)**2
    F(NEXP)=F(NEXP)+R1*R4
    R(NEXP+IRST)=R(NEXP+IRST)+S6*R1*R3
    RL(NEXP,NEXP)=RL(NEXP,NEXP)-R1*R3
    JCB(NEXP,NEXP)=JCB(NEXP,NEXP)-R1*R3
54  LGL=(KPEN.GE.0.0.OR.NEXP.GT.NSTAR(KS)).AND.(NEXP.NE.1)
    DO 56 J=1,NL
    S4=S1*R4*BETA(J)
    IF(LGL) JCB(NEXP,J)=JCB(NEXP,J)-R1*S4
56  IF(LGL) JCB(1,J)=JCB(1,J)+S4
    IF(.NOT.LGL) GO TO 82
    RL(1,1)=RL(1,1)-R2
    JCB(1,1)=JCB(1,1)-R2
    F(1)=F(1)-R4
    R(1+IRST)=R(1+IRST)+S6*R2
    EMET=EMET-S2*Q
    GO TO 90
60  IF(LPRNT) WRITE(6,111)
    LPRNT=.FALSE.
    IF(KPEN.GE.0.0) GO TO 50
    LGP=.FALSE.
    WRITE(6,112)
    GO TO 90
70  Q=1.0/DS(1+LN)**2
    R2=ANMET*ABS(KPEN)
    R4=ABS(KPEN)/ANEP
    S3=2.0*ANPL
    IF(.NOT.(ZC.LT.ZS)) S3=S3-ANC(NCORE)
    S3=S5*S3
    IF(KPEN.LT.0.0) GO TO 74
72  S4=ANMET*ANR(1)-ANMEQ*S3
    RPEN=ANMET*ANR(1)-ANMEQ*S5*ANPL
    GO TO 78
74  IF(ZC.LT.ZS.OR.NEXP.EQ.NSTAR(KS)) GO TO 76
    KPEN=-KPEN
    NEXP=NSTAR(KS)
    GO TO 72
76  IS=NEXP-NSTAR(KS)
    IF(IS.LE.0) GO TO 86
    IF(IS.EQ.NSTAR(KS+1)) GO TO 79
    IS=MS+IS
    S3=2.0*ANB(IS)

```

```

RPEN=ANMET*ANR(1)-S5*ANMEQ*ANB(1S)
77 S4=ANMET*ANR(1)-S5*ANMEQ*S3
78 R4=S4*R4
ANMET=R4*BETA(1)
IF(NEXP.EQ.NSTAR(KS)) R4=R4-ANMEQ*QM*ABS(KPEN)/ANEP
IF(NEXP.EQ.(NSTAR(KS)+NSTAR(KS+1))) R4=R4-S5*ANMEQ*QM*
C ABS(KPEN)/(2.0*ANEP)
RPEN=ANEP*BETA(1)*RPEN*ABS(KPEN)
LGI=.FALSE.
ANMEQ=ANMEQ*BETA(1)
GO TO 54
79 IF(ZC.LT.ZS-1) GO TO 60
S3=3.0*ANHS-ANG(NCORE)
RPEN=ANMET*ANR(1)-S5*ANMEQ*ANHS
GO TO 77
80 R1=1.0/BETA(NEXP)
81 R2=ANEP*BETA(1)
R3=R2*ANMEQ*ABS(KPEN)
R4=ANMET
IF(NEXP.GE.NSTAR(KS)) GO TO 82
GO TO 53
82 EMET=EMET-S2*Q
ANMET=R2
ANMEQ=R1*ANMEQ
GO TO 90
86 R1=ANEP/S5
GO TO 81
90 CONTINUE
C END PENNING SOURCE CODE
J=1
IF(NCAV.LE.0) GO TO 96
92 CONTINUE
DO 94 K=1,NCAV
I=LC(K)
IF(I.NE.J) GO TO 94
J=J+1
GO TO 92
94 CONTINUE
96 IGMX=0
97 IF(J.GE.5) GO TO 100
IF(GP(1,J).GT.0.0) GO TO 98
GO TO 100
98 IF(IGMX.EQ.0) IGMX=J
IS=LU(1,J)
IS=LU(2,J)+IFN(IS,L)
GP(3,J)=PHI(IS)
J=J+1
GO TO 97
100 IF(NB.GE.NSTAR(KS)) GO TO 160
IS=NB-1
NV=NSTAR(KS)-NB
CALL INVERS(RL,BVS,NV,.TRUE.,F,$130)
DO 120 K=1,NV
ANB(K+MR)=-RL(K+IS,NPL)*ANPL
DO 120 J=1,IS
ANB(K+MR)=ANB(K+MR)-RL(K+IS,J)*ANB(J+IRST)
F(J)=F(J)-RL(J,K+IS)*F(K+IS)
RL(J,NPL)=RL(J,NPL)-RL(J,K+IS)*RL(K+IS,NPL)
DO 120 I=1,IS

```

```

120  RL(J,I)=RL(J,I)-RL(J,K+IS)*RL(K+IS,I)
      GO TO 135
130  WRITE(6,113)
133  LERR=.TRUE.
      GO TO 160
135  CALL INVERS(JCB,BVS,NV,.FALSE.,ANR,$150)
      DO 140 J=1,IS
        ANR(J)=BETA(J)
        DO 140 K=1,NV
          ANR(J)=ANR(J)-BETA(K+IS)*JCB(K+IS,J)
          JCB(J,NPL)=JCB(J,NPL)-JCB(K+IS,NPL)*JCB(K+IS,J)
        DO 140 I=1,IS
140  JCB(I,J)=JCB(I,J)-JCB(I,K+IS)*JCB(K+IS,J)
      GO TO 160
150  WRITE(6,114)
      GO TO 133
160  RETURN
C    IF NBAR IS LESS THAN NSTAR THE FOLLOWING SUBROUTINE IS USED IN
C    CALCULATING EFFECTS OF QUASI-STATIONARY LEVELS
      SUBROUTINE INVERS(AMS,BVS,NV,LOGC,F,$)
      LOGICAL LOGC
      REAL AMS(NLM,1),BVS(NV,1),F(NLM)
      DO 10 K=1,NV
        DO 10 J=1,NV
10     AM(J,K)=AMS(J+IS,K+IS)
        DO 20 J=1,NV
          DO 14 K=1,IS
14     BVS(J,K)=AMS(J+IS,K)
          IF(LOGC) BVS(J,NB)=AMS(J+IS,NPL)
20     IF(LOGC) BVS(J,NB+1)=F(J+IS)
          I=IS
          IF(LOGC) I=I+2
          CALL SOR(AM,NLM,NV,BVS,NV,I,$30,DW)
          GO TO 40
30     RETURN 6
40     DO 50 J=1,NV
          DO 44 K=1,IS
44     AMS(J+IS,K)=BVS(J,K)
          IF(LOGC) AMS(J+IS,NPL)=BVS(J,NB)
50     IF(LOGC) F(J+IS)=BVS(J,NB+1)
          RETURN
C    THE FOLLOWING SUBROUTINE CALCULATES FREQUENCY AVERAGED CAVITY
C    RATE FUNCTIONS NEGLECTING HOLE BURNING
      SUBROUTINE CAVITY(RC,RCP,G,X,P,CF)
      CF=CGM*P
      CK=(1.0-LPI(X))/(1.0+CF)
      S=-G/ALOG(CMR)
      ST=AMAX1(1.0-S,0.0)
      RC=FCAV*S*(1.0-CK*ST**0.3)
      ST=AMIN1(S,0.99)
      IF(S.LE.0.99) GO TO 20
      IF(S.GE.1.01) GO TO 10
      CK=CK*EXP(1.0E3*(ST-S))
      GO TO 20
10     CK=0.0
20     RCP=FCAV*S*(1.0-CK*(1.0-1.3*ST)/(1.0-ST)**0.7)
      RETURN
      END

```

Subroutine MATRIX is used to collect the results from calls to SRJM and form the overall rates and Jacobian. The argument list is as follows:

ANR	vector of dependent variables (lower level densities, photon densities, $d \ln T_e / dt$ ), input
FF	vector of lower level rates
DMJ	Jacobian matrix
BETA	vector of lower level Saha factors
ANEP	predicted $N_e$ input
ANP	vector of maximum ionization densities
GLTE, CGME, DGME	(see SRJM list).
DE	electron rate heating/ $kT_e$
LCD	input integer vector; total number of lower level equations of species with indices $< i$ is LCD( $i$ )
AN, EP, DI, DEL	(see CONSRV list)
LERR, CVP	(see SRJM list)
ANPH	photon density vector
FMD	vector of mode spacing parameters
CVT	same as CVOUT in SRJM (cavity outputs)
GOUT, LOUT	maximum positive noncavity gain outputs: GOUT(1,k) is gain logarithm, GOUT(2,k) is escape factor, LOUT(i,k) are level indices ( $i = 1$ lower, $i = 2$ upper) for ion or atom types k

In the subroutine DEM is the overall rate matrix. Also RPEN is the Penning rate constant rather than KPEN and PRATE is the net Penning rate rather than RPEN (see SRJM list). DPEN is the increment to the electron rate heating due to the Penning effect. At output, ANEP is the corrected electron density.

-TFOR,SI SUB17

```

SUBROUTINE MATRIX(ANR,FF,DMJ,BETA,ANEP,ANP,GLTE,CGME,DGME,DE,LCD,
C   AN,EP,DI,DEL,LERR,CVP,ANPH,FMD,CVT,GOUT,LOUT)
  INCLUDE SPEC1,LIST
  INCLUDE SPEC2,LIST
  INCLUDE SPEC4,LIST
  INCLUDE SPEC5,LIST
  INCLUDE SPEC6,LIST
  INCLUDE SPEC7,LIST
  PARAMETER NLL=NCM+1,NST1=3*KM*NPL,NST2=NST1+KM*KM,NST3=NST2+2*NHSQ
  PARAMETER N17S=KM+1,N17S2=N17S+KM,N17S3=N17S2+KM
  DIMENSION ANP(NCM),LCD(NLL),BETP(NLM),DEM(KM,KM),DMJ(KM,KM),
C   FF(KM),BETA(KM),GG(KM),H(KM),BTP(KM),RL(NLM,NPL),
C   AJB(NLM,NPL),F(NLM),LC(4),CVP(2,4),FMD(4),CVT(3,4),
C   GOUT(2,NSP),LCUT(2,NSP)
  LOGICAL LERR,LGP
  EQUIVALENCE (BETP(1),SV(1)),(GG(1),STRMTX(1)),(H(1),STRMTX(N17S)),
C (BTP(1),STRMTX(N17S2)),(F(1),STRMTX(N17S3)),(DEM(1,1),
C STRMTX(NST1)),(RL(1,1),STRMTX(NST2)),(AJB(1,1),STRMTX(NST3))
  MS=C
  IS=C
  DO 5 J=1,NC
    IF(J.EQ.NC) GO TO 1
    K2=IC(J+1)-1
    GO TO 2
1   K2=NSP
2   K1=IC(J)
    DO 5 K=K1,K2
      L=INDS(K+1)
      MI=NBAR(K)-1
      DO 3 I=1,MI
3     ANP(I+MS)=ANP(I+IS)
      IS=IS+MI
      MS=MS+L
5     CONTINUE
    DO 7 K=1,IS
      DO 7 J=1,IS
        DEH(J,K)=C.0
7     DMJ(J,K)=C.0
    CALL CONGRV(DPEN,ANP,EP,DI,DEL,GM,AN,C)
    B1=C.0
    B2=C.0
    B3=C.0
    DPEN=C.0
    R1=C.0
    R2=C.0
    LR1=C
    LR2=C
    LD1=C
    LD2=C
    MS=C
    IS=C
    DO 100 J=1,NC
      IF(J.EQ.NC) GO TO 31
      K2=IC(J+1)-1
      GO TO 51
31   K2=NSP
51   K1=IC(J)
      ZS=K2-K1+1

```

```

ANHS=ANP(J)
NEXP=0
L1=LCD(J)+1
L2=LCD(J+1)
DO 100 K=K1,K2
ZC=K-K1+1
IF(K.LT.K2) GO TO 61
BETAPL=1.0/ANEP
GO TO 71
61 L=INDS(K+1)
BETAPL=BT(MS+L+1)
71 LGP=.FALSE.
L=NBAR(K)-1
DO 81 I=1,L
BETA(I+IS)=BT(I+MS)
81 GG(I+IS)=ANEP*ANEP*(ZS-ZC+1.0)/QM
IF(.NOT.LPN) GO TO 40
PENNING SOURCE CODE - SET A
IPEN=C
IF(J.EQ.JRC.AND.K.EQ.K1) GO TO 10
IF(J.EQ.JRC.AND.K.EQ.K1+1) GO TO 20
IF(J.EQ.JDC.AND.K.EQ.K1) GO TO 30
GO TO 40
10 IPEN=1
RATIN=RPEN
LGP=.TRUE.
NEXP=JRL
IF(RPEN.LT.0.0) NEXP=NEXP+NSTAR(K)
L=IC(JDC)
I=INX(L,2)-1
EMCT=15.79/TE
EMET=EMET/DS(I+1)**2-EMET/DS(I+JDL)**2
L=L-1
MI=0
DO 12 I=1,L
12 MI=MI+INDS(I+1)
ANMET=ANEP*BT(MI+JDL)*ANB(MI+JDL)
ANMEQ=ANEP*BT(MI+JDL)*ANB(MI+1)
A1=ANEP*BT(MS+1)
ANGR=A1*ANB(MS+1)
IF(NEXP.LT.NSTAR(K)) ANUR=A1*ANB(MS+JRL)
IF(NEXP.EQ.NSTAR(K).AND.K.EQ.K2) ANUR=A1*ANHS
GO TO 40
20 IPEN=2
RATIN=RPEN
IF(NEXP.LT.NSTAR(K1)) GO TO 4
LGP=.TRUE.
NEXP=1
IF(RPEN.LT.0.0) GO TO 22
ANUR=A1*ANEP*BT(MS+1)*ANPL
GO TO 40
22 NEXP=JRL
IF(NEXP.EQ.NSTAR(K)) GO TO 24
ANUR=A1*ANB(MS+JRL)
GO TO 40
24 ANUR=A1*ANHS
GO TO 40
30 IPEN=3
RATIN=ABS(RPEN)

```

```

LGP=.TRUE.
PRATE=SAVE
NEXP=-JDL
EMET=0.0
IF(RPEN.LT.0.0) ANUR=ANMET*ANUR
ANMET=ANUR
ANMEQ=ANGR
C END SOURCE SET A
40 CONTINUE
CALL SRJM(RL,AJB,F,AI,AR,ARR,QCRI,QCRR,K,MS,AN,ANEP,QM,ANFH,
C ANHS,BETAPL,GLTE,CGME,DGME,ZS,ZC,ANPL,LC,CVP,LGP,J,NEXP,RATIN,
C PRATE,ANMET,ANMEQ,EMET,LERR,IGMX,FMD,CVT)
IF(LERR) GO TO 110
GOUT(1,K)=0.0
GOUT(2,K)=0.0
LOUT(1,K)=0
LOUT(2,K)=0
IF(IGMX.LE.0) GO TO 41
GOUT(1,K)=GP(1,IGMX)
GOUT(2,K)=GP(3,IGMX)
LOUT(1,K)=LU(1,IGMX)
LOUT(2,K)=LU(2,IGMX)
41 A2=K2+1-K
A3=ANEP*BETAPL*ANPL
B1=B1+A2*(ANEP*AI-A3*AR)
B2=B2+A2*A3*(ARR-AR)
IF(K.EQ.K2) B2=B2+AR*ANC(J)
B3=B3+A3*QCRR-ANEP*QCRI
L=NBAR(K)-1
DO 42 MI=1,L
BTP(MI+IS)=BTP(MI)
H(MI+IS)=-F(MI)
IF(K.EQ.K2) H(MI+IS)=H(MI+IS)+QM*RL(MI,NPL)/A
42 GG(MI+IS)=GG(MI+IS)*BTP(MI)
DO 50 MI=1,L
IF(K.LT.K2) GO TO 46
FF(MI+IS)=RL(MI,NPL)*ANP(J)
DO 44 NI=L1,L2
44 DMJ(NI+IS,NI)=-RL(MI,NPL)*ANEP*BTP(NI)
GO TO 48
46 FF(MI+IS)=0.0
DEM(MI+IS,L+1+IS)=RL(MI,NPL)
DMJ(MI+IS,L+1+IS)=RL(MI,NPL)
48 DO 50 NI=1,L
DEM(NI+IS,MI+IS)=RL(NI,MI)
DMJ(NI+IS,MI+IS)=DMJ(NI+IS,MI+IS)+AJB(NI,MI)
50 CONTINUE
NI=LCD(NC+1)
A3=A2*ANEP
A2=A2*AR
DO 60 I=1,NI
IF(K.LT.K2) GO TO 54
DO 52 MI=L1,L2
52 DMJ(I,MI)=DMJ(I,MI)-ANR(I)*A2*ANEP*BTP(MI)
GO TO 56
54 DMJ(I,L+1+IS)=DMJ(I,L+1+IS)+A2*ANEP*BETAPL*ANR(I)
56 IF(I.GT.IS.AND.I.LE.IS+L) GO TO 60
DO 58 MI=1,L
DMJ(I,MI+IS)=DMJ(I,MI+IS)-ANR(I)*A3*AJB(MI,NPL)

```



```

58 CONTINUE
60 CONTINUE
IF(.NOT.LPN) GO TO 99
C PENNING SOURCE CODE - SET B
IF(IPEN.GT.0) GO TO (70,80,90),IPEN
GO TO 98
70 IF(LGP) GO TO 72
LPN=.FALSE.
GO TO 99
72 A2=0.0
A3=0.0
A4=0.0
SAVE=PRATE/ANEP**2
LR1=IS+1
LR2=IS+JRL
IF(RPEN.LT.0.0) LR2=LR2+L
IF(RPEN.GE.0.0.AND.JRL.GE.NBAR(K1).OR.RPEN.LT.0.0.AND.
C JRL.GE.NBAR(K1+1)) LR2=0
IF(NEXP.GE.NSTAR(K1)) GO TO 73
R1=SAVE
ANMET=SAVE
GO TO 76
73 R1=ANMET
IF(RPEN.LT.0.0.AND.NEXP.LT.NSTAR(K1)+NSTAR(K1+1)) GO TO 74
IF(RPEN.GE.0.0.AND.K1.EQ.K2) A2=RPEN
IF(RPEN.LE.0.0) A2=ANEP*BETAPL*ABS(RPEN)/2.0
A2=A2*ANMEQ*QM/ANEP
A3=SAVE
74 SAVE=ANMET-A2
ANMET=ANMET+A3
76 R2=ANMET
IF(JRL.EQ.NSTAR(K1+1).AND.RPEN.LT.0.0.OR.JRL.EQ.NSTAR(K1).AND.
C K1.EQ.K2) GO TO 78
GO TO 79
78 R2=0.0
A4=ANMEQ*ANEP*ABS(RPEN)
IF(RPEN.LT.0.0) A4=A4*ANEP*BETAPL
79 IF(RPEN.LT.0.0.OR.K1.LT.K2) GO TO 98
80 DPEN=EMET*PRATE
GO TO 98
90 LD1=IS+1
LD2=IS+JDL
IF(JDL.GE.NBAR(K1)) LD2=0
GO TO 98
96 DO 97 I=L1,L2
IF(J.EQ.JRC) DMJ(LR1,I)=DMJ(LR1,I)+A4*BTP(I)/BETA(LR1)
IF(J.EQ.JDC) DMJ(LD1,I)=DMJ(LD1,I)-A4*BTP(I)/BETA(LD1)
IF(J.EQ.JDC.AND.LD2.GT.0)DMJ(LD2,I)=DMJ(LD2,I)+A4*BTP(I)/BETA(LD2)
97 CONTINUE
GO TO 99
98 IF(K.EQ.K2.AND.NEXP.NE.0) GO TO 96
C END SOURCE SET B
99 IS=IS+L
100 CONTINUE
IS=0
NI=LCD(NC+1)
DO 104 K=1,NSP
L=NBAR(K)-1
DO 102 MI=1,L

```

```

J=MI+IS
A3=0.0
77-11 |
IF(J.EQ.LR1) A3=R1/BETA(LR1)
IF(J.EQ.LR2) A3=-R2/BETA(LR2)
IF(J.EQ.LD1) A3=-R1/BETA(LD1)
IF(J.EQ.LD2) A3=R1/BETA(LD2)
DO 102 I=1,NI
IF(I.GT.IS.AND.I.LE.IS+L) GO TO 102
DMJ(J,I)=DMJ(J,I)+(H(J)+A3)*GG(I)
102 CONTINUE
104 IS=IS+L
CALL CONSRV(ANEP,ANP,EP,DI,DEL,QM,AN,1)
CGME=B1
DGME=B1+B2
DE=B3*ANEP+DPEN
DO 106 J=1,NI
DO 106 K=1,NI
106 FF(J)=FF(J)+DEM(J,K)*ANR(K)
110 RETURN
END

```

Function TMSA is used to calculate the spontaneous emission factor for the cavity. (DM is the mode spacing parameter.)

Subroutine EICP calculates electron-ion collision parameters according to the results of Ref. 26. (see also Refs. 1 and 5.) The ratio of collision integrals  $B_{ei}^*$  is not explicitly used in the program and is set equal to a nominal value of unity. Argument Z is the ion charge number.

Subroutine ELEN calculates  $d\ln T_e/dt$  at a given time TAU (see argument lists of SRJM, MATRIX). The electron energy equation is discussed in Refs. 1 and 5. Input forcing functions are given by FORIN in the following manner: output BM is the magnetic field intensity (nominally null), IDIS is an integer that defines the type of forcing function, FT is  $T_e$  and FP is  $d\ln T_e/dt$  if  $IDIS \leq 0$ , FT is the total electric field tangent to the magnetic field and FP is the perpendicular electric field if  $IDIS = 1$  and FT, FP are the component current densities if  $IDIS > 1$ . The dummy subroutine calls ADUMYn are to be replaced by subroutines giving electron-atom collision parameters (elastic cross section Q and collision integral ratios B\* and C\*). Nominal (final) variables in TEMPS common are: H, H1, H3 - Hall parameters (see references), SIGMA - electrical conductivity, ALPHT - thermal diffusion ratio, FEC - electron-heavy particle elastic energy exchange collision frequency, Q - joule dissipation (units of  $10^8 \text{ Jm}^{-3} \text{ sec}^{-1}$ ) and QR - continuum radiation (MKS units if multiplied by  $5.4 \times 10^5$ ).

-TFOR,SI SUB18

FUNCTION TMSA(ETA,PS,DM,CL,CAR,WL)

TMSA=ETA

RETURN

END

-TFOR,SI SUB19

SUBROUTINE EICP(TE,ANE,Z,QEI,BEI,CEI)

BEI=1.0

DL=864.88\*SQRT(TE/ANE)

TS=0.151\*DL\*TE/Z

IF(TS.LE.1.0) GO TO 10

DL=DL/TS

QEI=DL\*DL\*ALOG(3.0\*TS)

TS=TS\*\*0.2

CEI=0.351\*TS/(TS-0.325)

RETURN

10 QEI=1.0986\*DL\*DL/TS

CEI=0.52

RETURN

END

```

SUBROUTINE ELEN(GLTE,TAU,DE,CGME,AN,ANP)
  INCLUDE SPEC1,LIST
  INCLUDE SPEC2,LIST
  DIMENSION CSTR(8),A(2,2),F(2),TN(2),AN(NSP),ANP(NCM)
  EQUIVALENCE (A(1,1),CSTR(1)),(TN(1),CSTR(5)),(F(1),CSTR(7))
  EQUIVALENCE (TMP(21),CSTR(1)),(TMP(29),S),(TMP(30),Q),(TMP(31),B)
  C      (TMP(32),C),(TMP(33),ALPHT),(TMP(34),DEL),(TMP(35),H1),
  C      (TMP(36),H3),(TMP(37),H),(TMP(38),SIGMA),(TMP(39),FEC),
  C      (TMP(40),QR),(TMP(41),Z),(TMP(42),AM)
  CALL FORIN(TAU,DIS,BM,FT,FP)
  IF(DIS.LE.0) GO TO 20
  H=15.79/TE
  QR=0.0
  FEC=0.0
  DO 1 J=1,8
1  CSTR(J)=0.0
  DO 10 J=1,NC
  IF(J.EQ.NC) GO TO 2
  K2=IC(J+1)-1
  GO TO 3
  2  K2=NSP
  3  K1=IG(J)
  H1=K2-K1
  DO 8 K=K1,K2
  Z=K-K1
  I=INX(K,1)+1
  AM=DS(I)
  C=DS(I+2)
  IF(K.LT.K2) S=AN(K+1)
  IF(K.EQ.K2) S=ANP(J)
  I=INX(K,2)+NSTAR(K)-1
  Q=(Z+1.0)/(DS(I)-0.5)
  QR=QR+S*C*(Z+1.0)**4*EXP(H*Q*Q)
  S=AN(K)
  IF(K.GT.K1) GO TO 6
  I=1
  C  DUMMY SUBR CALLS ARE TO BE CONVERTED BY COLLECTOR
  IF(J.EQ.1) CALL ADUMY1(TE,Q,B,C)
  IF(J.EQ.2) CALL ADUMY2(TE,Q,B,C)
  IF(J.EQ.3) CALL ADUMY3(TE,Q,B,C)
  IF(J.EQ.4) CALL ADUMY4(TE,Q,B,C)
  IF(J.EQ.5) CALL ADUMY5(TE,Q,B,C)
  IF(J.EQ.6) CALL ADUMY6(TE,Q,B,C)
  GO TO 7
  6  I=2
  CALL EICP(TE,ANE,Z,Q,B,C)
  7  IN(I)=TN(I)+S
  S=Q*S
  F(I)=F(I)+S
  FEC=FEC+S/AM
  A(1,I)=A(1,I)+B*S
  A(2,I)=A(2,I)+C*S
  IF(ABS(H1-Z).GT.0.5) GO TO 8
  Z=H1+1.0
  S=ANP(J)
  GO TO 6
  8  CONTINUE
  10 CONTINUE

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DO 12 K=1,2
S=F(K)
DO 12 J=1,2
12 A(J,K)=A(J,K)/S
S=F(2)/F(1)
Q=1.0+S
B=1.0+0.7*S-0.48*A(1,1)
C=1.2*(A(2,1)+S*A(2,2))-Q.
ALPHT=C/B
DEL=ALPHT*C/Q
H1=SQRT(TE)
QR=ANE*QR/H1
FEC=FEC*H1
H1=H1*(F(1)+F(2))
SIGMA=3.402E3*ANE/H1
H1=2.1233E3*BM/H1
H3=0.4*H1*Q/B
Q=DEL/(1.0+H3*H3)
H=H1+Q*H3
Q=1.0-Q
H=H/Q
DEL=1.0-DEL
IF(IDIS.EQ.1) Q=SIGMA*(FT*FT/(Q*(1.0+H*H))+FP*FP/DEL)
IF(IDIS.GT.1) Q=(Q*FT*FT+DEL*FP*FP)/SIGMA
GLTE=DE/(1.5*ANE)+(4.829E-3*Q-2.6085E-5*QR)/(ANE*TE)-9.088E-4*
C   FEC*(TE-T)/TE-CGME
GO TO 30
20 TE=FT
GLTE=FP
30 RETURN
END

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