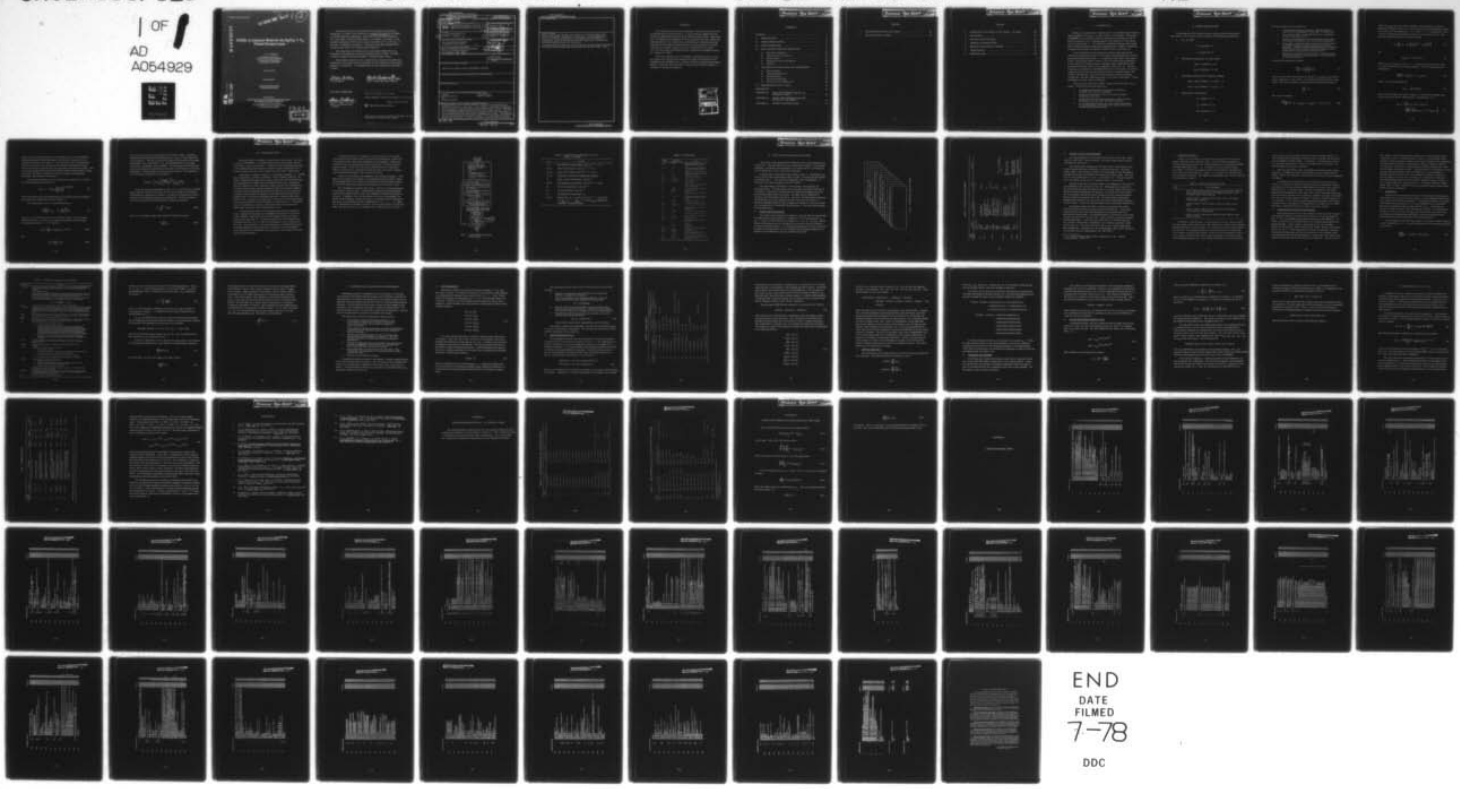
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SPIKE: A Computer Model for the $H_2(D_2) + F_2$ Pulsed Chemical Laser

J. J. T. HOUGH

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14 April 1978

Interim Report

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This report has been reviewed by the Information Office (OI) and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nations.

This technical report has been reviewed and is approved for publication. Publication of this report does not constitute Air Force approval of the report's findings or conclusions. It is published only for the exchange and stimulation of ideas.

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A comprehensive rate equation model for a pulsed laser pumped by the $H_2(D_2)$-F_2 reaction is described. This computer simulation incorporates up to 216 kinetic reactions to describe the laser medium, which is assumed to be homogeneous and contained in a Fabry-Perot optical cavity. The first fifteen vibrational-rotational P-branch transitions from each of the lowest ten vibrational bands are monitored for possible laser action. The distinctive features incorporated in this model include: (1) the elimination of the gain-equals-loss assumption, so that it is possible to predict cavity transients

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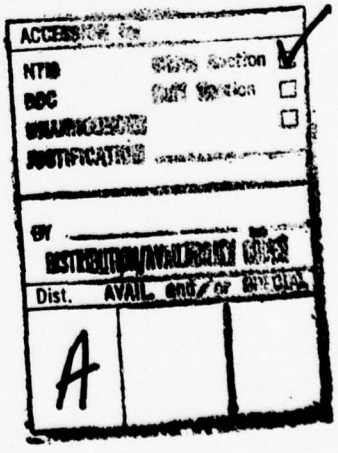
and to observe gain-intensity interactions; (2) a detailed model of the Lorentz broadening, including V, J dependence, as well as distinction between various perturbing species; (3) multiquantum HF(DF) self-deactivation, which in the HF case was found important to achieve good agreement between theory and experiment.

Comparisons of the prediction of this model with several small-scale experiments have indicated generally good agreement (typically within ~20%).

PREFACE

The preliminary work in the development of this code was carried out at Michigan State University with R. L. Kerber and was supported by the Division of Engineering Research of the College of Engineering. Subsequent work, including the incorporation of the D_2-F_2 kinetics and the comparisons with experiments, was carried out at The Aerospace Corporation and was supported by the Defense Advanced Research Projects Agency, the Naval Sea Systems Command, and the Air Force Weapons Laboratory under U.S. Air Force Space and Missile Systems Organization (SAMSO) Contract No. F04701-77-C-0078.

This code originally was not intended for distribution; hence, it may not contain some convenience measures that might be desirable from the standpoint of the unfamiliar user. Sufficient detail is provided in this report, however, such that, with some effort, the user will be able to modify the program for his specific purposes.



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I. INTRODUCTION

SPIKE, a comprehensive computer model of the HF(DF) pulsed chemical laser pumped by the $H_2(D_2) + F_2$ chain reaction, is described. This model incorporates up to 216 kinetic reactions and takes into detailed account the effects of pressure line-broadening based on the results of a recent survey of the literature (Ref. 1). The method of computation utilized in this model did not require the gain-equals-loss assumption and is capable of predicting transients and relaxation oscillations within the laser cavity (Ref. 2).

Recent comparisons of the predictions of this model with several small-scale pulsed H_2-F_2 laser ($\sim$25-cm gain length) experiments revealed generally good agreement (Ref. 2). Comparisons with larger scale experiments ($\sim$100-cm gain length), however, have not shown as good agreement in the prediction of absolute energy, although relative performance with parameter variations still showed comparable results (Ref. 3). This lack of agreement is indicative of possible deficiencies in the model. It has been suggested that such phenomena as photoionization, photodissociation, and medium nonuniformity, which have been neglected in typical modeling calculations, may have significant impact on the larger scale lasers. These possibilities are still under investigation.

Several recent requests for SPIKE, reflect the need for this "users guide." The objectives in this report are:

1. To explain the theories from which the calculations executed in the code are formulated.
2. To present in systematic form the formal and logical structures of the code.
3. To describe the procedures necessary in order to obtain information from this code with minimal lag time.
4. To provide sufficient detail such that, with some preparation, modifications to the code can be made so that it can be tailored to particular needs.

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II. MODEL FORMULATION

The formulation of the chemical laser computer model is described in this section. The reactions used to represent the chemical processes are:

1. $H_2 + F_2$ chain

$$F + H_2 \rightleftharpoons HF(v) + H$$

$$H + F_2 \rightleftharpoons HF(v) + F$$

2. Vibrational-translational (VT) deactivation

$$HF(v) + M \rightleftharpoons HF(v') + M$$

$$H_2(v) + M \rightleftharpoons H_2(v - 1) + M$$

3. Vibrational-vibrational (VV) quantum exchange

$$HF(v) + HF(v') \rightleftharpoons HF(v + 1) + HF(v' - 1)$$

$$HF(v) + H_2(v') \rightleftharpoons HF(v + 1) + H_2(v' - 1)$$

4. Dissociation-recombination

$$F_2 + M \rightleftharpoons M + F + F$$

$$H_2 + M \rightleftharpoons M + H + H$$

$$HF + M \rightleftharpoons M + H + F$$

The major features in the models are:

1. The dominant kinetic processes are represented by the reaction system suggested by Cohen (Ref. 4) (Table A-1).
2. The reacting mixture is homogeneous and is contained in a Fabry-Perot laser cavity.
3. The rotational populations for each vibrational level have a Boltzmann distribution at the translational temperature.
4. All possible transitions within a band are assumed to have low initial intensities that grow if the gain rises above threshold. Lasing is always assumed to be in the P-branch. Initial intensity levels can be selected individually or set proportional to the spontaneous emission rate.
5. Initiation is modeled by the introduction of a finite concentration of F atoms into the gas mixture, or through the use of a flash-lamp option.

The chemical reactions are written

$$\sum_i \alpha_{ri} N_i \underset{k_{-r}}{\overset{k_r}{\rightleftharpoons}} \sum_i \beta_{ri} N_i \tag{1}$$

where N_i is the molar concentration of species i, α_{ri} and β_{ri} are stoichiometric coefficients, and k_r and k_{-r} are forward and backward rate coefficients. The rate of change of concentration for nonlasing molecules is

$$\frac{dN_i}{dt} = X_i \tag{2a}$$

and, for HF molecules,

$$\frac{dN_{HF(v,J)}}{dt} = X_i + X_{rad}(v, J) - X_{rad}(v - 1, J_L) + A(v, J) \tag{2b}$$

where the X_{rad} terms are rates of change in concentration as a result of lasing into and out of level (v, J). The lower-level rotational quantum numbers are J and J_L for the transitions $v + 1 \longrightarrow v$ and $v \longrightarrow v - 1$, respectively. The net rate of spontaneous emission into level (v, J) is given by A(v, J). The chemical reactions yield a concentration change

$$X_i = \sum_r (\beta_{ri} - \alpha_{ri}) \left(k_r \prod_j N_j^{\alpha_{rj}} - k_{-r} \prod_j N_j^{\beta_{rj}} \right) \tag{3}$$

and

$$X_{rad}(v, J) = g(v, J)\, f(v, J) \tag{4}$$

where g(v, J) is the gain on the $v + 1 \longrightarrow v$ transition with lower level J and f(v, J) is the lasing flux on the same transition. The rate equation for the lasing flux is

$$\frac{df(v, J)}{dt} = c\left(\frac{L}{\ell}\right) [g(v, J) - \alpha_{thr}] f(v, J) \tag{5}$$

where c is the speed of light and

$$\alpha_{thr} = -\frac{1}{2L} \ln(R_o R_L) \tag{6}$$

where L is the length of the active medium, ℓ is the mirror spacing, and R_o and R_L are the mirror reflectivities. The gain (Ref. 5) is

$$g(v, J) = \frac{hN_A}{4\pi} \omega_c(v, J)\, \phi(v, J)\, B(v, J) \times \left[\left(\frac{2J + 1}{2J - 1} \right) N_{HF(v+1,\, J-1)} - N_{HF(v,\, J)} \right] \tag{7}$$

where $\omega_c(v, J)$ is the wave number of the transition, $B(v, J)$ is the Einstein isotropic absorption coefficient based on the intensity, and $\phi(v, J)$ is the Voigt profile at line center (Ref. 6). The first term of Eq. (5) determines the rate of increase in the intensity of the radiation field within the laser cavity; the second term gives the rate energy that is lost from the cavity. The lost energy includes that extracted through the output coupler as laser output, as well as real losses resulting from such mechanisms as absorption, scattering, and extraneous reflections.

A Boltzmann distribution at the translational temperature (T) is taken for the rotational populations; hence,

$$N_{HF(v, J)} = N_{HF(v)} \left(\frac{2J + 1}{Q_r^v(T)} \right) e^{-hcE_J^v/kT} \tag{8}$$

where the values of the rotational partition function $Q_r^v(T)$ and the rotational energy E_J^v are computed from Mann et al. (Ref. 7).

The energy equation for a constant density gas is

$$\frac{dT}{dt} \sum_i N_i C_{v_i} = -P_L - \sum_i \frac{dN_i}{dt} H_i \tag{9}$$

where C_{v_i} is the molar specific heat at constant volume, H_i is the molar enthalpy of species i, and P_L is the output lasing power per unit volume. The output power in the $v + 1 \longrightarrow v$ band is

$$P_{Lv}(t) = \sum_j hc\, N_A \alpha_{thr} \omega_c(v, J) f(v, J) \tag{10a}$$

and

$$P_L(t) = \sum_v P_{Lv}(t) \tag{10b}$$

where the only cavity loss is assumed to be the laser output. In making comparisons with experimental measurements, however, real losses must be accounted for. One way to do this is to assume that fraction of the output attributable to the "total reflector" R_L (as distinguished from the output coupler R_o) corresponds to cavity losses. The transmissivity of the mirror (R_L) may be adjusted to approximate cavity losses resulting from scattering, transmission, and absorption at various optical surfaces. The useful fraction of the total output power is then (Ref. 6)

$$P_{useful} = \frac{P_{total}(1 - R_o)}{[1 + (R_o/R_L)^{1/2}][1 - (R_o/R_L)^{1/2}]} \tag{11}$$

From the numerical integration of Eqs. (2), (5), and (9) by the modified Adams-Moulten method of Gear (Ref. 8), the time evolution of the species concentrations, temperature, pressure, the gain on all transitions, and the intensities on all lasing transitions are determined. The laser energy extracted in each band is then determined by integrating the power

$$E_v = \int_0^{t_c} P_{Lv} dt \tag{12a}$$

where t_c is the length of laser pulse and the total pulse energy is

$$E = \sum_v E_v \tag{12b}$$

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III. CODE DESCRIPTION

The broad features of SPIKE are described in this section. The code is written in FORTRAN. A complete listing of the main program and the subroutines is given in Appendix C. In addition to the explanations provided in this and the subsequent sections, extensive comment statements are included throughout the body of the listing to provide further clarification.

The program consists of a main (or controlling), program, i.e., SPIKE, and six subroutines: INPUT1, LORENTZ, GAIN, DIFSUB, DIFFUN, and RATE. SPIKE obtains input data by calling subroutine INPUT1 and initiates such computational variables as concentration, photon flux, temperature and time; defines the cavity conditions; obtains reaction rate constants and necessary spectroscopic and thermodynamic data from data files; updates the pressure line-broadening parameters through the use of the subroutine LORENTZ; and provides the program control parameters that direct the program flow, as well as the integration process. Subroutine (function) GAIN is used to compute the medium gain of the laser for any given allowed vibrational-rotational P-branch transition by means of Eq. (7). The photon fluxes corresponding to the seven transitions within each band with the highest gain are monitored for possible laser action.

Time progression within the model proceeds along the integration steps. Numerical integration is accomplished through the use of the subroutine DIFSUB, which utilizes the modified Adams-Moulten technique presented by Gear (Ref. 8). Derivatives required for the integration are computed from Eqs. (2), (5), and (8) and obtained by means of subroutine DIFFUN. Laser initiation by electrical discharge (or flash photolysis) may be modeled through a flash-lamp option contained in the main program, which provides a time-dependent F-atom production rate based on the input power (intensity) profile.

Substantial savings in computation time and computer core storage requirements were obtained with the present code formulation, wherein the rate equations were input as an integral part of the program, and the rate coefficients were precomputed and stored on disk for retrieval during program execution. In the event that minor modifications to the rates are desired, rather than re-creating the entire rate file, these minor changes are accomplished through the use of subroutine RATE.

Figure 1 is a schematic flow diagram of the computer program. This figure is an overview of the chain of commands and decisions used to obtain the integrated values of the species concentrations within the laser medium, as well as the laser power density and temperature as a function of time.

The variables and symbols used in Fig. 1 and in the computer program are defined in Tables 1 and 2. Bookkeeping limitations and computational practicability demand that the many time-dependent variables be grouped in an array. In addition, since the dimension of an array is changeable, the model has the flexibility to alter the number of variables under consideration. The array is two dimensional and is designated $Y(I, J)$, $J = 1, \ldots, N$, where $Y(1, J)$ represents the variable in question, N is the total number of such variables, and $Y(I, J)$ and $I > 1$, are related to the $(I - 1)$th derivatives of $Y(1, J)$.

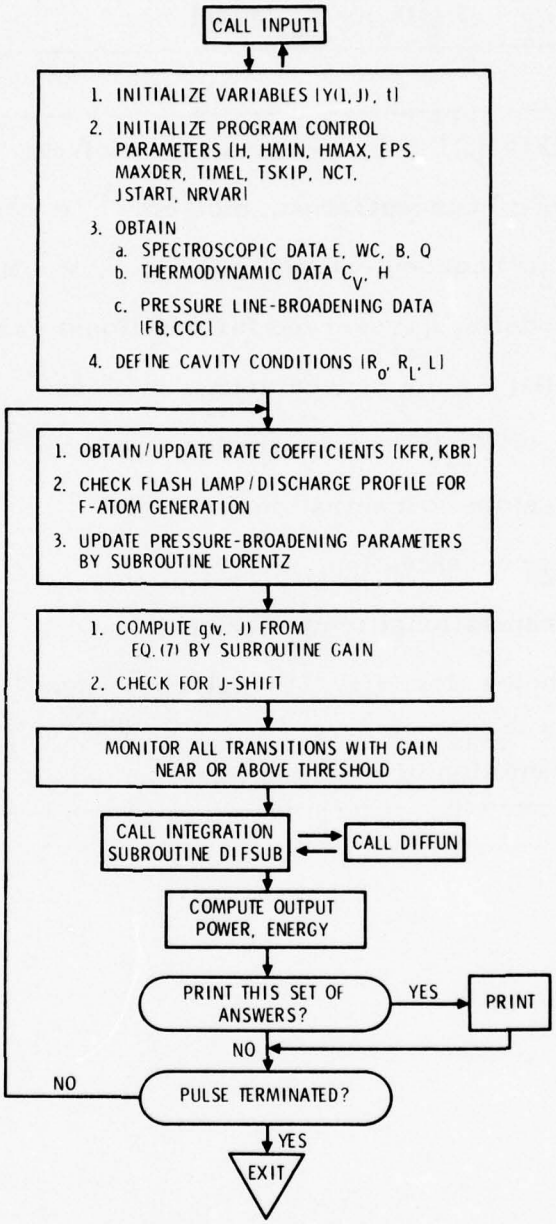


Fig. 1. Pulsed HF(DF) Chemical Laser Model

Table 1. Identification of Variables Y(1, N) in $H_2(D_2) + F_2$ Model

N	Y(1, N)
1-9	HF(v)[DF(v)] concentration, mol-cm^{-3}, v = N-1
10-11	DF(v) concentration, mol-cm^{-3}, v = N-1
12-14	N_2(v) concentration, mol-cm^{-3}, v = N-12
15-16	Undefined, reserved for additional variables
17	H(D) - atom concentration, mol-cm^{-3}
18-20	H_2(v)[D_2(v)] concentration, mol-cm^{-3}, v = N-18
21	F-atom concentration, mol-cm^{-3}
22	F_2 concentration, mol-cm^{-3}
23	Translational temperature, K
24-79	Photon flux, f(v, J), mol-cm^{-2}-sec^{-1}, v = $\lvert$(N-17)/7$\rvert$, J = J^v_{max} - 4, . . . , J^v_{max} + 2, where J^v_{max} indicates the transition of maximum gain.

Table 2. Nomenclature

Symbol in Text	Symbol in Computer Program	Definition
$A(v, J)$	A(V, J)	Einstein isotropic coefficient for spontaneous emission, 1/molecule-sec
$B(v, J)$	B(V, J)	Einstein isotropic intensity absorption coefficient, cm^2/molecule-J-sec
c	C	Speed of light, 2.997925×10^{10} cm/sec
C_{V_i}	CVI	Molar specific heat at constant volume of species i, cal/mol-K
E_J^v	E(V, J)	Rotational energy of state V, J, cm^{-1}
$f(v, J)$	FLUX(V, J)	Photon flux, mol-cm^{-2}-sec^{-1}
$g(v, J)$	ALPHA(V, J)	Gain of transition $(v + 1, J - 1) \rightarrow (v, J)$, cm^{-1}
h	-	Planck's constant, 6.6256×10^{-34} J-sec
h	-	Specific enthalpy, kcal/g
H_i	EHPY!	Molar enthalpy of species i, kcal/mol
I	CRRNT	Discharge current, A
k	K	Boltzmann's constant, 1.38054×10^{-23} $J\text{-}K^{-1}$
k_r, k_{-r}	KFR, KBR	Forward and backward rate constants, in terms of moles, centimeters, and seconds
L	LNTH	Length of active medium, cm
N_i	Y(1, I)	Concentration of species i, mol-cm^{-3}
dN_i/dt	DERV1Y(I)	Time derivative of N_i, mol-cm^{-3}-sec^{-1}
N_A	NA	Avogadro's number, 6.02252×10^{23} molecules-mol^{-1}
P_L	POWER	Power density of laser output, W-cm^{-3}
P_I	PIN	Power input from initiation, W-cm^{-3}
Q_r^v	Q(V, T)	Rotational partition function for level v
$R_O R_L$	RO, RL	Mirror reflectivities
R	R	Universal gas constant, 1.98725 cal-mol^{-1}-K^{-1}
t	T	Time, sec
T	Y(1, 23)	Temperature, K
α_{ri}, β_{ri}	-	Stoichiometric coefficients of reaction r
α_{thr}	THGAIN	Threshold gain, cm^{-1}
$\phi(v, J)$	PHI(V, J)	Normalized line profile of transition $(v + 1, J - 1) \rightarrow (v, J)$, cm
τ_R	TAU(V, J)	Rotational relaxation time constant, sec
$\omega_c(v, J)$	WC(V, J)	Wave number of transition $(v + 1, J - 1) \rightarrow (v, J)$, cm^{-1}

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IV. BASIC INSTRUCTIONS FOR USING SPIKE

The common input preparations needed for most runs are discussed in this section. The input parameters are classified as follows: (1) initial gas conditions, (2) optical cavity parameters, (3) output control, (4) integration control parameters, and (5) initiation mechanism.

A sample set of input data cards is shown in Fig. 2. The proper location for these cards is immediately after the end-of-record card that follows the program decks. This format corresponds to that of NAMELIST. A summary of the input variables is given in Table 3.

The input data are divided into seven groups; each group has an identifying name. The data stream for each group is initiated by the sign $ in Column 2, followed by the group name (no blank must appear between $ and the group name) and then the data. The data must be separated by commas, and terminated by another $. However, the data within each group can be listed in any order and may extend to more than one record. It should be emphasized that no data can appear in Column 1 of any one record, as it is ignored by the NAMELIST READ operation. The seven data streams are described below.

A. INITIAL GAS CONDITIONS

The initial concentrations of the species in the gas mixture are provided through the data stream SPECIES. In addition to the reacting species F_2, H_2, F, and H, several diluents are modeled, i.e., He, Ar, N_2, SF_6, and O_2. These concentrations may be provided in any units (but must be consistent) or simply as relative ratios. An initial HF(0) population may also be entered. Pressure of the gas mixture in Torr (PRESS) and initial gas temperature in degrees kelvin (TEMP) are input by the data stream GAS.

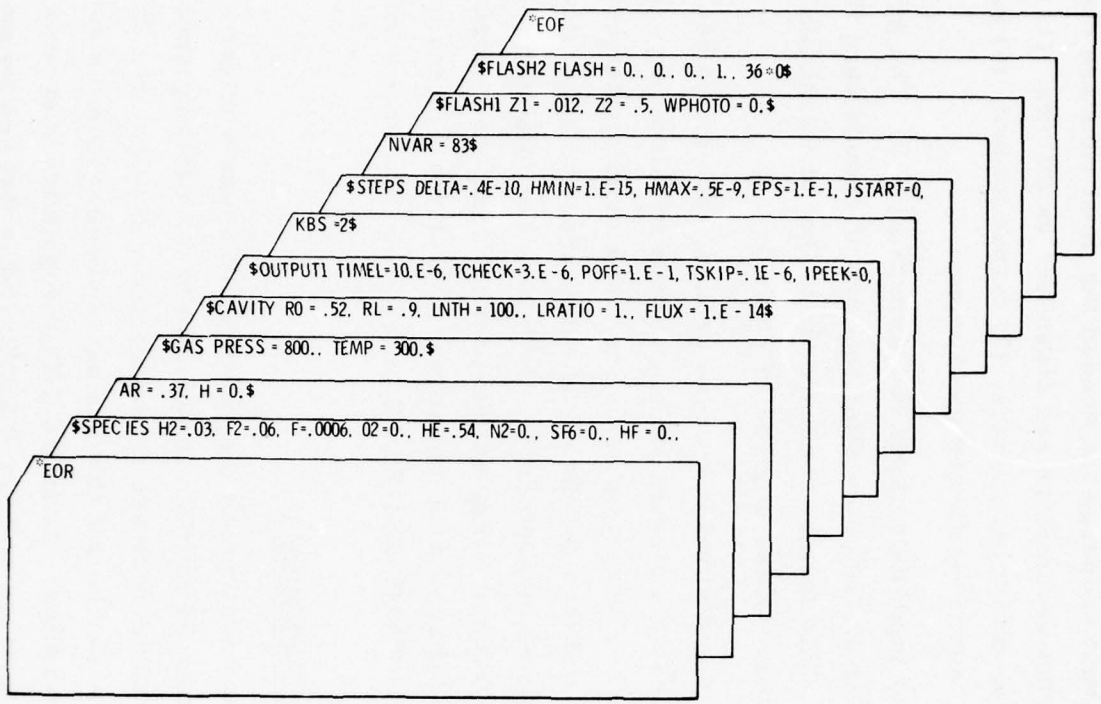


Fig. 2. Sample Input Data for SPIKE

Table 3. Summary of Input Variables

Group Name	Variable	Definition	Units	Comments
SPECIES	H_2, F_2, F, H, He, Ar, N_2, O_2, HF, SF_6	Species concentrations	Arbitrary	
GAS	PRESS	Total gas pressure	Torr	
	TEMP	Gas temperature	Kelvin	
CAVITY	R0	Output coupler reflectivity	-	
	RL	Mirror reflectivity	-	
	LNTH	Medium gain length	cm	
	LRATIO	Ratio of gain length to mirror separation	-	
	FLUX	Initial photon flux	mol/cm^2-sec	
OUTPUT1	TIMEL	Upper limit of integration	sec	
	TCHECK	Check for pulse termination at t > TCHECK	sec	
	POFF	Power density at termination	W/cm^3	
	TSKIP	Time between prints	sec	
	IPEEK	Controls limited print option	-	IPEEK = {0, Full print; 1, Limited print}
	KBS	Printout format selector	-	$1 \leq KBS \leq 5$
STEPS	DELTA	Initial step size	sec	See Table 5 for more complete information
	HMIN	Minimum step size	sec	
	HMAX	Maximum step size	sec	
	EPS	Error test constant		
	JSTART	Input indicator		
	NVAR	Number of integration variables		
FLASH1	Z1	Peak flash lamp output	mol/cm^3	FLASH1 and FLASH2. Data are not needed if flash option not used.
	Z2	Defined by Eq. (14)		
	WPHOTO	Average energy of absorbed photon	cm^{-1}	
FLASH2	FLASH(2, 20)	I(1), t(1), I(2), t(2), . . . , I(20), t(20)	I = nondimensional t = sec	It is not required to use all 40 elements in this array.

B. OPTICAL-CAVITY PARAMETERS

The input parameters for the laser optical cavity are R0, RL, LNTH, LRATIO, and FLUX. These quantities, contained in data stream CAVITY, are defined in this section.

The optical cavity is assumed to be Fabry-Perot, with mirror reflectivities denoted by R0 and RL and given in decimal fractions. R0 is the output coupler, and only that fraction of the total radiant energy that passes through this mirror is included in the calculation of laser output. Note that the "0" in the symbol R0 is a "zero," not the letter "O." The gain length of the active medium is given by the variable LNTH in centimeters.

LRATIO is the ratio of the gain length to the separation of the mirrors, corresponding to the L/ℓ factor in Eq. (5). This parameter accounts for the intervals during which the photons traverse regions between the mirrors, which are neither amplifying nor absorbing. The larger the "null" region, the fewer passes each photon makes through the active medium during the photon residence time within the cavity. This phenomenon reduces the amplification potential of the cavity and can result in appreciable reduction in laser output. It has been observed experimentally at Sandia Laboratories.[1]

All possible transitions within a band are assumed to have initial intensity levels that grow if the gain rises above threshold. These initial intensity levels can be selected individually or set proportional to the spontaneous emission rate. Our standard practice has been to set all initial intensity levels at 10^{-14} mol/cm^2-sec, which is done by setting the variable FLUX to this value. Test cases where this value was varied by as much as $\times 10^3$ have indicated the calculations to be relatively insensitive to this number (Ref. 2). The value of FLUX is set to zero to make small signal gain calculations. (Alternatively, the threshold gain value can be increased to any large number by adjusting R0, RL, and LNTH.)

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[1] J. B. Moreno, Sandia Laboratories, Albuquerque, N.M., private communication, April 1977.

C. OUTPUT CONTROL

TSKIP, KBS, and IPEEK are three input parameters that control the quantity and form of the computer output. As the calculation progresses, pertinent data are printed at time intervals specified by the parameter TSKIP (seconds) beginning at time t = 0. A final print is also obtained at pulse termination. Contents of the printed output are controlled by the parameter KBS, which may have values of $1 \leq KBS \leq 5$. The larger the value selected, the more print is obtained. The outputs corresponding to the various values of KBS are shown in Table 4.

Table 4. Definition of Parameter KBS

KBS	Printed Output
1	Time, laser power, laser energy, gas temperature, species concentrations, total number of integration steps to reach this time, and the last step size.
2	Output of KBS = 1 plus the photon flux, power, and energy of each laser transition.
3	Output of KBS = 2 plus the gain of each transition at this time.
4	Output of KBS = 3 plus the self-broadening coefficients $\gamma(v, J)$ and other linewidth data.
5	Output of KBS = 4 plus rate coefficients and reaction rates for all reactions.

In addition to printed output, an array (XXX) is written, which contains the laser power, laser energy, time, gas temperature, species concentrations, and gain and power of each transition. At each print interval, XXX is copied onto Tape 13. The parameter KKK is incremented each time to keep track of the number of times XXX is copied. At the end of the calculation, Tape 13 may be saved, either for later use in a plotting program or for a brief scan of the calculated results (e.g., this file may be quickly retrieved and studied

on an interactive terminal while the main output is waiting to print). If only the abbreviated output data contained in XXX is needed, the main print may be skipped by setting IPEEK = 1 (otherwise, it should be set to zero). The resulting output will be two prints corresponding to the initial (t = 0) and final (pulse termination) conditions.

The input data TSKIP, KBS, and IPEEK are punched in data stream OUTPUT1. In addition to these, this data stream also contains the data TIMEL, POFF, and TCHECK, which determine the point at which computation is stopped.

Termination of the calculation occurs with the onset of one of two events: (1) integration reaches an imposed time limit specified by TIMEL (seconds) or (2) the power density drops below some preset level, given by POFF(W/cm^3). In the latter case, to avoid terminating the calculation during the developing phase of the laser power, this terminating mechanism does not become operative until an interval, TCHECK (seconds), has elapsed. The user must provide values for TIMEL, TCHECK, and POFF as part of the input data. In the case of a small-signal-gain calculation, where power remains at zero, termination of computations is controlled only by TIMEL. The value of TCHECK should be set larger than that of TIMEL.

D. INTEGRATION CONTROL PARAMETERS

Numerical integration of the rate equations within the present model is accomplished utilizing a modified Adams-Moulten technique presented in Ref. 8. The corresponding integration subroutine is called DIFSUB. The reader is referred to the original reference for details regarding this integration package. Under ordinary circumstances, only the variables NVAR(=N), DELTA(=H), HMIN, HMAX, EPS, YMAX, KFLAG, and JSTART will be of concern. NVAR represents the number of integration variables contained in the program, DELTA is the step size to be attempted on the next integration step, HMIN and HMAX are, respectively, the minimum and maximum step sizes that will be used for the integration. EPS is an error

test constant, which represents the maximum error (estimate) that can be tolerated on a step; it is expressed as a "fraction" of the maximum value (YMAX) of each integration variable (Y) seen up to this point in the integration. The user also has the option of adjusting the values of YMAX to influence the step sizes. KFLAG is an output flag from DIFSUB that gives the result of the previous integration attempt. A KFLAG value of +1 indicates a successful step, whereas a negative value corresponds to an unsuccessful one. JSTART defines the action on the next integration attempt: to repeat the previous step, to continue with a new step, or to indicate the first step. A more detailed description of these and other variables is given in Table 5; the contents of which are taken from Ref. 8. The value of DELTA, HMIN, HMAX, EPS, JSTART, and NVAR must be provided through the data stream STEPS to make a calculation.

E. INITIATION

Initiation of the chemical reactions is either through an instantaneous introduction of F atoms into the gas mixture or a time-dependent dissociation of F_2 molecules by a flash-lamp option. If the flash-lamp option is selected, input values for the parameters Z1, Z2, and WPHOTO must be provided, along with a flash-lamp output intensity profile (I vs t). These data are entered by means of data streams FLASH1 and FLASH2. For instantaneous initiation, on the other hand, the user need only provide an initial F-atom concentration in the data stream SPECIES, neglecting the data streams associated with the flash-lamp option FLASH1 and FLASH2.

The formulation of the flash-lamp option in the present model is similar to that in RESALE (Ref. 6). The rate of dissociation of the absorbing species n_a is given by

$$\left(\frac{dn_a}{dt}\right)_{f\ell} = -Z_1 I(t)\left[1 - \exp(-Z_2 n_a)\right] \qquad (13)$$

Table 5. Definition of Parameters in DIFSUB

Parameter	Definition
N = NVAR	The number of first-order differential equations. N may be decreased on later calls if the number of active equations reduces, but it must not be increased without calling with JSTART = 0.
T	The independent variable.
Y	An 8 by N array containing the dependent variables and their scaled derivatives. Y(J + 1, I) contains the J-th derivative of Y(I) scaled by H**J/factorial(J) where H is the current step size. Only Y(1, I) need be provided by the calling program on the first entry. If it is desired to interpolate to non-mesh points, these values can be used. If the current step size is H and the value at T + E is needed, form S = E/H, and then compute $$Y(I)\ (T + E) = \sum_{J=0}^{NQ} Y(J + 1, I) * S^{**}J$$
SAVE	A block of at least 12*N floating point locations used by the subroutines.
H = DELTA	The step size to be attempted on the next step. H may be adjusted up or down by the program in order to achieve an economical integration. However, if the H provided by the user does not cause a larger error than requested, it will be used. To save computer time, the user is advised to use a fairly small step for the first call. It will be automatically increased later.
HMIN	The minimum step size that will be used for the integration. Note that on starting this must be much smaller than the average H expected since a first-order method is used initially.
HMAX	The maximum size to which the step will be increased.
EPS	The error test constant. Single-step error estimates divided by YMAX(I) must be less than this in the Euclidean norm. The step and/or order is adjusted to achieve this.
MF	The method indicator. The following are allowed: 0 An Adams predictor corrector is used. 1 A multi-step method suitable for stiff systems is used. It will also work for non-stiff systems. However, the user must provide a subroutine PEDERV which evaluates the partial derivatives of the differential equations with respect to the Y's. This is done by call PEDERV(T, Y, PW, M). PW is an N by N array which must be set to the partial of the I-th equation with respect to the J dependent variable in PW(I, J). PW is actually stored in an M by M array where M is the value of N used on the first call to this program. 2 The same as Case 1, except that this subroutine computes the partial derivatives by numerical differencing of the derivatives. Hence PEDERV is not called.
YMAX	An array of N locations which contains the maximum of each Y seen so far. It should normally be set to 1 in each component before the first entry (See the description of EPS.)
ERROR	An array of N elements which contains the estimated one-step error in each component.
KFLAG	A completion code with the following meanings: +1 The step was successful. -1 The step was taken with H = HMIN, but the requested error was not achieved. -2 The maximum order specified was found to be too large. -3 Corrector convergence could not be achieved for H .GT. HMIN. -4 The requested error is smaller than can be handled for this problem.
JSTART	An input indicator with the following meanings: -1 Repeat the last step with a new H. 0 Perform the first step. The first step must be done with this value of JSTART so that the subroutine can initialize itself. +1 Take a new step continuing from the last. JSTART is set to NQ, the current order of the method at exit. NQ is also the order of the maximum derivative available.
MAXDER	The maximum derivative that should be used in the method. Since the order is equal to the highest derivative used, this restricts the order. It must be less than 8 or 7 for Adams or stiff methods, respectively.
PW	A block of at least N**2 floating point locations.

where n_a is the concentration (mol/cm^3) of the absorbing species. Values for Z_1, Z_2, ω_ν, and a flash-lamp profile I(t) must be provided. Z_1 is the peak flash-lamp output in moles per unit volume of gas. Z_2 is defined by the relation

$$Z_2 = \frac{\alpha_\nu \ell}{n_a} \frac{cm^3}{mole} \tag{14}$$

where α_ν is the absorption coefficient of species n_a in a gas container of mean geometric length ℓ. ω_ν (WPHOTO) is the average energy of the absorbed photon in cm^{-1}.

Z_1, Z_2, and WPHOTO are input by means of the data stream FLASH1, and the flash-lamp output intensity profile is input by the data stream FLASH2. The format for the flash-lamp intensity profile is as follows:

$$\$FLASH2\ FLASH = I(1),\ t(1),\ I(2),\ t(2), \ldots,\ I(20),\ t(20)$$

where I(k) is the flash output intensity at time t(k). I(k) is nondimensional, and its peak value is normalized to unity.

As shown in Appendix B, for an optically thin gas mixture, the initiation level through photodissociation of F_2 reduces to the approximate expression

$$\frac{[F]}{[F_2]} \cong 2 Z_1 Z_2 \tag{15}$$

For such cases, Z_2 can be set equal to one-half to obtain

$$\frac{[F]}{[F_2]} \approx Z_1 \tag{16}$$

This approximation provides an alternative technique for simulating flash-lamp initiation, which, under certain conditions, may be easier to apply. As an example, suppose parametric calculations must be made in which it is desired to vary the flash-lamp profile but maintain the same initiation level. With this technique, after setting Z_1 to the desired initiation level, and Z_2 to one-half, all that is needed for each new run is a new flash-lamp profile. This procedure is certainly easier than using Eq. (13) directly. It should be remembered, however, that in applying the above approximation the flash profile is normalized in a different sense. In the "exact" treatment i.e., Eq. (13), the peak flash value is set to unity, whereas, in the optically thin approximation case, the profile is normalized by

$$\int_0^\infty I(t)\, dt = 1 \qquad (17)$$

V. CHANGING RATE EQUATIONS AND COEFFICIENTS

Substantial savings in computation time and computer core storage requirements were obtained with the present code formulation, wherein the rate equations were input as an integral part of the program and the rate coefficients were precomputed and stored on disk for retrieval during program execution. The drawback of this economy measure is that changes in rate equations or rate coefficients can require a rather significant effort. The economy gained, however, is believed to justify this inconvenience. The procedure for making these changes is described in this section.

The basic steps involved in making these changes follow:

1. New variables must be defined and initialized. The total number of integration variables is represented by the variable NVAR, which should be adjusted to reflect this change.
2. New reactions must be incorporated into subroutine DIFFUN, and the derivatives affected by these reactions updated to reflect the changes.
3. The thermodynamic properties of any new species introduced must be incorporated in the input data. The new species must also be considered in the gas temperature calculations.
4. Pressure-broadening effects contributed by the new species may not be negligible, in which case, the calculation for the Lorentz half-half width must be revised.
5. Rate modifications are made in the rate data files. Rate coefficients corresponding to new reactions must be added to these data files.
6. Format can be modified if desired.

A detailed description is given for the addition of oxygen-related kinetics to the code to illustrate the procedure. The reactions and rate constants utilized are essentially those compiled by Taylor et al. (Ref. 9) and given in Table 6. The deactivation of HF(v) by O_2 is taken to be similar to that by N_2, reduced by a factor of 3 (Ref. 10).

A. NEW VARIABLES

Several new species are introduced in these reactions: O, O_2, H_2O, OH, HO_2, and FO_2. As indicated in Section III, the variables in this program are represented by elements in any array Y(1, N), N = 1, ..., 100. At this point, the locations corresponding to N = 15, 16, and 80 through 100 are unreserved. Therefore, the new variables may be assigned to any of these positions. In this example, the concentrations of these species will be represented as follows:

$$\begin{aligned} Y(1,15) &= [O] \\ Y(1,16) &= [O_2] \\ Y(1,80) &= [OH] \\ Y(1,81) &= [H_2O] \\ Y(1,82) &= [FO_2] \\ Y(1,83) &= [HO_2] \end{aligned} \tag{18}$$

For more efficient execution, it is best to keep the array dimension to a minimum. Thus, whereas a value of N up to 100 is possible, the present example was selected to occupy only up to N = 83. A smaller array may then be utilized for the program calculations. The input variable NVAR was implemented to help accomplish this purpose. NVAR designates the maximum size of the variable array that is to be used in the accompanying computation. Therefore, in the present situation,

$$NVAR = 83 \tag{19}$$

The new variables must also be initialized, i.e., assigned an initial value. A zero value will be automatically assigned unless otherwise instructed. It is assumed for the present purposes that only $Y(1, 16) = [O_2]$ has a nonzero value.

The following procedure may be used to introduce O_2 as a new input variable.

1. Expand the NAMELIST group SPECIES in the subroutine INPUT1 to include the variable O2.
2. Add O2 to GASSUM in the subroutine INPUT1. The fractional value of O2 is then computed by the statement:

$$O2 = O2/GASSUM$$

3. Add O2 to the common block GAS1, found in both the main program and subroutine INPUT1. Note that in this example, the variable name O2 was changed to RO2 in the main program.
4. Calculate the initial O_2 concentration (in moles/cm^3) in the main program by the statement

$$Y(1, 16) = RO2*FCTR \qquad (20)$$

where FCTR represents the appropriate conversion factor.

The location of these new statements, and others to be described below, are given in the listings in Appendix C. The changes described here are indicated in the listings by the symbol O_2.

B. DIFFUN MODIFICATIONS

The no-oxygen version of the code incorporates 150 kinetic reactions, designated by the reaction numbers shown in Table A-1. The additional 14 reactions considered here will be designated by numbers 151 through 164, as indicated in Table 6. The variable NEQN (main program) should be set to 164 to reflect the increased number of reactions. For each of these reactions (K), the forward [RCTF(K)] and backward rates [RCTB(K)] must be computed. As an example, Reaction No. 151 is written as

$$RCTF(151) = (Y(1, 15)**2)*M12*KFR(151)$$

$$RCTB(151) = M12*Y(1, 16)*KBR(151) \qquad (21)$$

where it is recalled that Y(1, 15) and Y(1, 16) refer to the species concentrations of O and O_2, respectively. KFR(151) and KBR(151) correspond to the forward

Table 6. Oxygen Kinetics

Reaction No.	Reaction	Rate Constant (k)	
		$cm^3/mol\text{-}sec$	$cm^6/mol^2\text{-}sec$
151	$O + O + M_{12} \xrightarrow{k} O_2 + M_{12}$	$7.98 \times 10^{19}\ T^{-1.5}$	$M_{12} = 2.820,\ O_2$
152	$O + O + M_{13} \xrightarrow{k} O_2 + M_{13}$	$3.0 \times 10^{15}\ T^{-0.5}$	$M_{13} = N_2$
153	$H_2 + OH \xrightarrow{k} H_2O + H$	$2.29 \times 10^{13}\ e^{-5200/RT}$	
154	$H + O_2 \xrightarrow{k} OH + O$	$2.71 \times 10^{14}\ e^{-16600/RT}$	
155	$O + H_2 \xrightarrow{k} OH + H$	$1.2 \times 10^{13}\ e^{-9000/RT}$	
156	$H + O_2 + M_{14} \xrightarrow{k} HO_2 + M_{14}$	$6.17 \times 10^{14}\ e^{1600/RT}$	$M_{14} = M_3,\ O_2,\ 1.8\ H_2,\ 1.8\ H_2O$
157	$H + OH + M_{15} \xrightarrow{k} H_2O + M_{15}$	$4.72 \times 10^{16}\ e^{1850/RT}$	$M_{15} = M_3,\ 5.1\ H_2O$
158	$H + O + M_3 \xrightarrow{k} OH + M_3$	6.17×10^{16}	
159	$OH + O + M_3 \xrightarrow{k} HO_2 + M_3$	3.6×10^{14}	
160	$H_2O + O \xrightarrow{k} 2OH$	$4.22 \times 10^{13}\ e^{-18000/RT}$	
161	$H + HO_2 \xrightarrow{k} 2OH$	1.81×10^{13}	
162	$H + HO_2 \xrightarrow{k} H_2 + O_2$	6×10^{12}	M_3 = all species
163	$O + HO_2 \xrightarrow{k} OH + O_2$	6×10^{12}	
164	$F + O_2 + M_3 \xrightarrow{k} FO_2 + M_3$	1.8×10^{15}	

and backward rate coefficients, respectively, of Reaction No. 151, and M12 represents the "concentration" of the catalytic species O and O_2. In the definition of M12, the concentration of O was multiplied by 2.82 to account for the larger reaction cross section with O as the third body compared to O_2. Note that M12, along with other catalytic species, is defined at the beginning of this subroutine, and that all these "M" variables must be converted from fixed to floating variables by the "REAL" statement.

The subroutine DIFFUN will compute the "net forward rate" RF(151)

$$RF(151) = RCTF(151) - RCTB(151) \tag{22}$$

which is then used to calculate the contributions to the derivatives of each species involved in these reactions. The contributions of Reaction Nos. 1 through 150 have already been accounted for in the no-oxygen formulation. The contributions of Reaction Nos. 151 through 164 remain to be included. The reader can easily verify that these reactions will affect the concentrations of the following species:

$$\begin{aligned} [O] &= Y(1, 15) \\ [O_2] &= Y(1, 16) \\ [H] &= Y(1, 17) \\ [H_2] &= Y(1, 18) \\ [F] &= Y(1, 21) \\ [OH] &= Y(1, 80) \\ [H_2O] &= Y(1, 81) \\ [FO_2] &= Y(1, 82) \\ [HO_2] &= Y(1, 83) \end{aligned} \tag{23}$$

Consider as an example atomic oxygen Y(1, 15). Its concentration depends directly on Reaction Nos. 151, 152, 154, 155, 158, 159, 160, and 163. Thus, the derivative of Y(1, 15) is written

$$\begin{aligned} \text{DERV1Y(15)} = \text{DERV1Y(15)} &- 2.*[\text{RF(151)} + \text{RF(152)}] \\ &+ \text{RF(154)} - \text{RF(155)} - \text{RF(158)} - \text{RF(159)} - \text{RF(160)} \\ &- \text{RF(163)} \end{aligned} \qquad (24)$$

where the first term accounts for contributions from Reaction Nos. 1 through 150, normally computed in preceding sections of the subroutine, and subsequent terms reflect the contributions from Reaction Nos. 151 through 164. Similar equations can be written for the other species. Two comments should be made in regard to Eq. (24). First, the leading term on the right-hand side of this equation is not necessary in this instance since its value is zero; however, this situation is not universal, e.g., in the case of DERV1Y(21). Thus, this term is always suggested to reduce the possibility of errors resulting from oversights. Second, it is possible to gain some computational economy by performing many of the calculations in this equation separately, as portions are repeated in subsequent statements. But the economy gained is at the expense of clarity of the individual rate equations (derivatives) and further complicates the process involved in changing reactions. The choice made here is to preserve that clarity.

C. ENERGY EQUATION

The contributions of the added species to the terms of the energy Eq. (9) are discussed. The following program variables are used.

$$\text{CVSUM} = \sum_i N_i C_{V_i}$$

$$\text{ETHLPY} = \sum_i \frac{dN_i}{dt} H_i$$

where N_i, C_{V_i}, and H_i are, respectively, the concentration, molar specific heat at constant volume, and molar enthalpy of species i.

The values of C_{V_i} and H_i for each of the new species must be incorporated into the program data files (Section VI). The following statements may be used to update the values of the variables CVSUM and ETHLPY:

```
CVSUM = CVSUM + CVO(IT)*Y(1,15) + CVO2(IT)*Y(1,16)
              + CVOH(IT)*Y(1,80) + CVH2O(IT)*Y(1,81)
              + CVFO2(IT)*Y(1,82) + CVHO2(IT)*Y(1,83)

ETHLPY = ETHLPY + EHPYO(IT)*DERV1Y(15)
                + EPHYO2(IT)*DERV1Y(16)
                + EHPYOH(IT)*DERV1Y(80)
                + EHPYH2O(IT)*DERV1Y(81)
                + EHPYFO2(IT)*DERV1Y(82)
                + EHPYHO2(IT)*DERV1Y(83)
```

For dilute mixtures where O_2 concentrations are small (e.g., $\sim$0.5%), the effect of these species on the energy equation, as well as on pressure broadening (as discussed in the following paragraphs), is not appreciable. Under these circumstances, the modifications suggested in steps C and D may be neglected with very little error.

D. PRESSURE BROADENING

The foreign-gas broadened linewidth is calculated in subroutine GAIN. The Lorentz half-half width is represented by the variable LONTZ. Hence, the concentration and pressure-broadening coefficients of the new species must be incorporated into the computation of the value of this variable. For the present, only O_2 will be considered.

The collision-broadening characteristics of HF vibrational-rotational transitions by O_2 are not available. However, from published HCl pressure-broadened linewidth data (Ref. 11), it may be justifiably assumed that the O_2 characteristic is similar to that of H_2 or D_2. The collision broadening of HF lines by O_2 is taken to be the same as H_2 in the present example. Thus, the following substitution is made in the statement that computes LONTZ:

$$\text{H2SUM} \longrightarrow \text{H2SUM} + \text{Y(1, 16)}$$

where H2SUM is the total H_2 concentration and Y(1, 16) is the O_2 concentration. This modification will result in a calculated Lorentz half-half width that accounts for the O_2 contribution.

E. RATE-COEFFICIENT MODIFICATION

As stated previously, the rate coefficients KFR and KBR used in equations such as Eq. (21) were precomputed and stored, either on a magnetic tape or on a disk, or both. The rate coefficients are taken to be of Arrhenius form, i.e.,

$$\begin{aligned} \text{KFR} &= A_{fr} T^{B_{fr}} e^{E_{fr}/RT} \\ \text{KBR} &= A_{br} T^{B_{br}} e^{E_{br}/RT} \end{aligned} \tag{25}$$

KFR and KBR are connected by the relation

$$K_r = (RT)^{\nu_r} \frac{\text{KFR}}{\text{KBR}} \tag{26}$$

where K_r is the equilibrium constant of the reaction, and

$$\nu_r = \sum_i \nu_{ri} = \sum_i (\beta_{ri} - \alpha_{ri}) \tag{27}$$

where α_{ri} and β_{ri} are stoichiometric coefficients of reaction r, as defined in Eq. (1). The equilibrium constant K_r is a function of temperature only and is given by

$$\ln K_r = - \frac{1}{RT} \sum_i \nu_{ri} H_i + \frac{1}{R} \sum_i \nu_{ri} S_i \tag{28}$$

where H_i (cal/mole) and S_i (cal/mole-K) are, respectively, the molar enthalpy and molar entropy of species i. The values of H_i and S_i may be obtained from the JANAF thermodynamic data compilation (Ref. 12).

The generation of the rate coefficient data files is accomplished through a separate program, RATE. (Note that this is not the subroutine RATE.) This program computes, from input data, the forward and backward rate coefficients at 25-K intervals from 100 to 6000 K. The input data consist of one card for each reaction, which specifies the values of A_{fr}, B_{fr}, E_{fr}, A_{br}, B_{br}, and E_{br} in the order given. The format used is

FORMAT (E15.8, F9.5, E16.8, E15.8, F9.5, E16.8)

The rate coefficients are calculated in this program using Eq. (25). The generated data are copied onto the logical files TAPE7 (KBR) and TAPE12 (KFR), which are subsequently saved for future use by the model SPIKE.

Under certain conditions, a simpler procedure may be followed to obtain the needed rate coefficients. For the present example, the deactivation rate of HF(v) by O_2 was taken to be similar to that by N_2, except that it was reduced by a factor of 3. Thus, the simulation of O_2 deactivation can be

easily accomplished by adding one-third of the O_2 concentration to the reactions that govern HF(v) deactivation by N_2, which is accomplished in the subroutine DIFFUN by adjusting the definition of M11 to:

$$M11 = SF_6 + N_2 + 0.3*Y(1, 16)$$

where Y(1, 16) is the element in the variable array that corresponds to the O_2 concentration. The rate coefficients for HF deactivation by N_2 are presently computed in subroutine RATE. Thus, to ensure that this subroutine is exercised, the following statement should be inserted in the main program:

```
IF(RO2.GT.0.) CALL RATE (Y(1, 23))
```

where RO2 refers to the O_2 ratio in the initial gas mixture.

VI. DESCRIPTION OF DATA FILES

In addition to the rate coefficients contained in data files TAPE7 and TAPE12, the program must have access to spectroscopic and thermodynamic data that relate to the species in the reacting gas mixture. These are summarized in Table 7. The data are punched into data cards following the formats indicated in the table and input by means of program DATA, which reads the data and stores them at predetermined locations (indicated by the tape numbers).

Most of the data files in the table need no explanation. The rotational energies E(v, J) and transitional wave numbers WC(v, J) are computed from the data of Refs. 7 and 13. The rotational partition function can then be computed from the equation

$$Q(v, T) = 1 + \sum_{J=1}^{\infty} (2J + 1) \exp\left(- \frac{hc}{k} \frac{E(v, J)}{T}\right) \tag{29}$$

The Einstein absorption coefficient is computed from the relation

$$B(v, J) = \frac{16\pi^4 \times 10^{-7}}{3h^2 c} \left(\frac{2J}{2J + 1}\right) \left| \mathcal{M}_{v, J}^{v+1,\ J-1} \right|^2 \tag{30}$$

where the matrix elements for the transitions $\mathcal{M}_{v, J}^{v+1,\ J-1}$ are from Meredith (Ref. 14). The heat capacity (CV) and enthalpy (EHPY) data are obtained from the JANAF thermodynamic data compilation.

The role of pressure broadening in the pulsed HF chemical laser is discussed in detail in Ref. 1. Self-broadened linewidths are calculated by the use of the data CCC. Foreign-gas broadening is based on the experimental data compiled in Ref. 1 and stored in array FB. The coefficients contained in the array CCC were calculated by Meredith (Ref. 15) on the basis of the

Table 7. SPIKE Input Data

Data Tape No.	Symbol	Definition	Format	Range	Units
1	E(v + 1, J + 1)	Rotational energy of state v, J	5E14.5	v = 0, ···, 9 J = 0, ···, 30	cm^{-1}
2	WC(v + 1, J)	Wave number of transition (v + 2, J + 1) ⟶ (v + 1, J)	5E16.5	v = 0, ···, 8 J = 1, ···, 18	cm^{-1}
3	B(v + 1, J)	Einstein isotropic intensity absorption coefficient of transition (v + 2, J + 1) ⟶ (v + 1, J)	5E16.5	v = 0, ···, 8 J = 1, ···, 18	$cm^{2}mol^{-1}$-J^{-1}-sec^{-1}
4	Q(v + 1, T + 1)	Rotational partition function for level v at temperature T × 100 K	5E16.5	v = 0, ···, 8 T = (0, ···, 60) × 100 K	
8[a]	$CV_i(T)$	Molar heat capacity at constant volume of species i (i = F, F_2, N_2, SF_6, H_2, HF) at temperature T × 100 K	5F16.5	T = (1, ···, 17) × 100 K	cal/mol-K
9[a]	$EHPY_i(T)$	Molar enthalpy of species i(i = H, H_2, F, F_2, HF) at temperature T × 100 K	5F16.5	T = (1, ···, 17) × 100 K	kcal/mol
14	CCC(I, K)	Pressure broadening coefficients for Kth band (see text for details)	7F10.5	I = 1, ···, 126 K = 1, ···, 10	$cm^{-1}atm^{-1}$
15	FB(J, K)	Foreign-gas broadened linewidth of transition (v + 1, J - 1) ⟶ (v, J) by species K, K = H_2, N_2, F_2, Ar, He, H, F, and SF_6, at 300 K	5F16.5	J = 1, ···, 15 K = 1, ···, 8	$cm^{-1}atm^{-1}$

[a]TAPE 8(9) contains the $CV_i(T)$ [$EPHY_i(T)$] arrays of the species in the order listed above.

Anderson theory for pressure broadening. The array is dimensioned CCC(126, 10), representing sets of 126 coefficients for each of 10 vibrational bands. These bands are: HF(0 - 1), HF(1 - 2), HF(2 - 3), HF(3 - 4), HF(4 - 5), DF(0 - 1), DF(1 - 2), DF(2 - 3), DF(3 - 4), and DF(4 - 5). Each set of 126 coefficients is additionally partitioned by means of an EQUIVALENCE statement into an array of the form C(7, 6, 3). The first index represents the seven coefficients needed for the equation

$$\gamma(m) = c_1 + c_2 e^{-m/4} + c_3 m e^{-m/4} + c_4 m^2 e^{-m/2} + c_5 m e^{-m^2/8} + c_6 m^2 e^{-m^2/16} + c_7 e^{-m^2/8} \quad (31)$$

which is the expression used by Meredith to represent the results of his Anderson theory calculation. In Eq. (31), m corresponds to the rotational quantum number for the lower level of the transition and $\gamma(m)$ is the Lorentz half linewidth at half maximum ($cm^{-1}atm^{-1}$). The coefficients c_i depend on the nature of the perturbing species, as well as on the gas temperature. The second index of array C(7, 6, 3) designates six different possible perturbers: HF(0), HF(1), HF(2), DF(0), DF(1), and DF(2). The third index represents the three temperatures for which the coefficients are given: 300, 600, and 900 K. For calculations of linewidth at temperatures other than these, linear interpolations and extrapolations are presently used.

The foreign-gas pressure broadening coefficients stored in the array FB(15, 8) correspond to the fifteen vibrational-rotational transitions modeled for each band and eight possible perturbing molecules: H_2, N_2, F_2, Ar, He, H, F, and SF_6. These coefficients were obtained experimentally at sample gas temperatures of ~300 K. At higher temperatures, a $\gamma(m) \sim T^{1/2}$ dependence is assumed for the present calculations, based on a hard sphere interaction model (Ref. 1).

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APPENDIX A

RATE COEFFICIENTS FOR $H_2 + F_2$ CHEMICAL LASER

The chemical kinetic model used for the rate-equation solution has been suggested by Cohen (Ref. 4) and is shown in Table A-1. Rate coefficients k and k_- designate forward and backward rates, respectively. For each reaction, the missing rate coefficient is determined from the equilibrium constant.

Table A-1. Rate Coefficients for $H_2 + F_2$ Chemical Laser[a]

Reaction No.	Reaction	Rate Coefficient, cm^3 mol-sec	M, v
11	$F + H_2(0) = HF(1) + H$	$k_{11} = 2.6 \times 10^{13-1.6/\theta}$	
12	$F + H_2(0) = HF(2) + H$	$k_{12} = 8.8 \times 10^{13-1.6/\theta}$	
13	$F + H_2(0) = HF(3) + H$	$k_{13} = 4.4 \times 10^{13-1.6/\theta}$	
14	$F + H_2(0) = HF(4) + H$	$k_{14} = 7.4 \times 10^{12-0.50/\theta}$	
15	$F + H_2(0) = HF(5) + H$	$k_{15} = 1.1 \times 10^{13-0.51/\theta}$	
16	$F + H_2(0) = HF(6) + H$	$k_{16} = 1.9 \times 10^{13-0.56/\theta}$	
17	$H + F_2 = HF(0) + F$	$k_{17} = 1.1 \times 10^{12-2.4/\theta}$	
18	$H + F_2 = HF(1) + F$	$k_{18} = 2.5 \times 10^{12-2.4/\theta}$	
19	$H + F_2 = HF(2) + F$	$k_{19} = 3.5 \times 10^{12-2.4/\theta}$	
20	$H + F_2 = HF(3) + F$	$k_{20} = 3.6 \times 10^{12-2.4/\theta}$	
21	$H + F_2 = HF(4) + F$	$k_{21} = 1.6 \times 10^{13-2.4/\theta}$	
22	$H + F_2 = HF(5) + F$	$k_{22} = 3.6 \times 10^{13-2.4/\theta}$	
23	$H + F_2 = HF(6) + F$	$k_{23} = 4.8 \times 10^{13-2.4/\theta}$	
24	$H + F_2 = HF(7) + F$	$k_{24} = 5.5 \times 10^{12-2.4/\theta}$	
25	$H + F_2 = HF(8) + F$	$k_{25} = 2.5 \times 10^{12-2.4/\theta}$	
26-41	$HF(v) + M_1 = HF(v') + M_1$	$k_{26-41} = v^{1.3}(10^{14.0}\, T^{-0.8} + 10^{0.4}\, T^{3.5})$	$M_1 = HF$, $v = 1 \cdots 8$, $v' < v$
42	$HF(1) + M_2 = HF(0) + M_2$	$k_{42} = 1.5 \times 10^{10-1.1/\theta}\, T$	$M_2 = F$
43	$HF(2) + M_2 = HF(1) + M_2$	$k_{43} = 1.5 \times 10^{10-0.5/\theta}\, T$	
44-49	$HF(v) + M_2 = HF(v - 1) + M_2$	$k_{44-49} = 1.5 \times 10^{10}\, T$	$v = 3 \cdots 8$
50-57	$HF(v) + M_4 = HF(v - 1) + M_4$	$k_{50-57} = (8 \times 10^{-4}\, T^4)v$	$M_4 = Ar, F_2$; $v = 1 \cdots$

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Table A-1. Rate Coefficients for $H_2 + F_2$ Chemical Laser[a] (Continued)

Reaction No.	Reaction	Rate Coefficient, cm^3 mol-sec	M, v
58-93	$HF(v) + M_6 = HF(v') + M_6$	$k_{58-93} = 1.8 \times 10^{13-0.7/\theta}$	M_6 = H, v = 1 · · · 8, $v' < v$
94-101	$HF(v) + M_5 = HF(v - 1) + M_5$	$k_{94-101} = v(8.7 \times 10^{-7}\ T^5)$	M_5 = He, v = 1 · · · 8
102-109	$HF(v) + M_7 = HF(v - 1) + M_7$	$k_{102-109} = v(1 \times 10^5\ T^2)$	$M_7 = H_2$, v = 1 · · · 8
110-116	$HF(v) + HF(v) = HF(v - 1) + HF(v + 1)$	$k_{110-116} = 1.5 \times 10^{12}\ T^{1/2}$	v = 1 · · · 7
118-123	$HF(v) + HF(v + 1) = HF(v - 1) + HF(v + 2)$	$k_{118-123} = 0.5k_{4a}$	v = 1 · · · 6
125-129	$HF(v) + HF(v + 2) = HF(v - 1) + HF(v - 3)$	$k_{125-129} = 0.25k_{4a}$	v = 1 · · · 5
131-134	$HF(v) + HF(v + 3) = HF(v - 1) + HF(v + 4)$	$k_{131-134} = 0.125k_{4a}$	v = 1 · · · 4
135	$HF(0) + H_2(1) = HF(1) + H_2(0)$	$k_{135} \approx 9 \times 10^{11}$	
136	$HF(1) + H_2(1) = HF(2) + H_2(0)$	$k_{136} \approx 2.9 \times 10^{12}$	
137	$HF(2) + H_2(1) = HF(3) + H_2(0)$	$k_{137} = 9 \times 10^{12}$	
138	$HF(3) + H_2(1) = HF(4) + H_2(0)$	$k_{138} = 2 \times 10^{13}$	
139	$HF(0) + H_2(2) = HF(1) + H_2(1)$	$k_{139} = k_{5a}$	
140	$HF(1) + H_2(2) = HF(2) + H_2(1)$	$k_{140} = k_{5b}$	
141-142	$H_2(v) + M_8 = H_2(v - 1) + M_8$	$k_{141-142} = v(2.5 \times 10^{-4})\ T^{4.3}$	v = 1, 2, M_8 = all except H, H_2
	$H_2(v) + M_9 = H_2(v - 1) + M_9$	$k_{141-142} = v(10^{-3}\ T^{4.3})$	v = 1, 2, M_9 = H, H_2
143-150	$HF(v) + M_{11} = HF(v - 1) + M_{11}$	$k_{143-150} = v^{2.5}(11\ T^3 + 2.4 \times 10^9)$	v = 1, · · · 8 $M_{11} = N_2$, SF_6,

[a] Note that dissociation-recombination reactions have been neglected.

[b] θ = 4.575 T/1000 kcal/mol

[c] v = vibrational level; M = collision partner

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APPENDIX B

FLASH-LAMP FORMULATION FOR OPTICALLY THIN GASES

For an optically thin gas mixture, the approximation

$$\exp(-Z_2 n_{F_2}) \cong 1 - Z_2 n_{F_2} \tag{B-1}$$

can be made. Thus, Eq. (29) can be written

$$\left(\frac{dn_{F_2}}{dt}\right)_{f\ell} \cong - Z_1 Z_2 n_{F_2} I(t) \tag{B-2}$$

Since two F atoms are introduced for every F_2 dissociated,

$$\left(\frac{dn_F}{dt}\right)_{f\ell} \cong 2 Z_1 Z_2 n_{F_2} I(t) \tag{B-3}$$

For low initiation levels, e.g., $F/F_2 \leq 2\%$, Eq. (B-3) can be integrated to obtain

$$\frac{[F]}{[F_2]} \cong 2 Z_1 Z_2 \int I(t)\, dt \tag{B-4}$$

where the notation $[F_2]$ was substituted for n_{F_2}. With a normalized intensity profile assumed, i.e.,

$$\int I(t)\, dt = 1 \tag{B-5}$$

$$\frac{[F]}{[F_2]} \cong 2\, Z_1 Z_2 \qquad \text{(B-6)}$$

is obtained. Thus, the quantity $2\, Z_1 Z_2$ is approximately the initiation level of the laser, and can be empirically set to the measured experimental value.

APPENDIX C

LISTING FOR MODEL SPIKE

```
      PROGRAM SPIKEHF(INPUT,OUTPUT,TAPE1,TAPE2,TAPE3,TAPE4,TAPE5,TAPE6,T
     1APE7=OUTPUT,TAPE9,TAPE10,TAPE11,TAPE12,TAPE13,TAPE14,TAPE15,TAPE8=
     2INPUT)
      DIMENSION Y(8,100), DERIV1Y(100), STORE(7), XXX(266)
      COMMON /DIFSUB/ YMAX(100),SAVE(12,100),ERROR(100),PW(10000)
      COMMON /SPECT/ E(10,31),WC(9,15),B(9,10),O(9,61)
      COMMON /CV/ CVH2(17),CVF(17),CVF2(17),CVHF(17),CVSF6(17),CVN2(17)
      COMMON /CVOXG/ CVO(17),CVO2(17),CVOH(17),CVH2O(17),CVH02(17)
      COMMON /EHPY/ EHPYH(17),EHPYF2(17),EHPYF(17),EHPYF2(17),EHPYHF(17)
      COMMON /EHPYOXG/ EHPYO(17),EHPYO2(17),EHPYOH(17),EHPYH2O(17),EHPYH
     102(17)
      COMMON /NUMVAR/ NVAR,NFVAR,NFLAG,MFLAG,NEQN
      COMMON /GAIN/ ALPHA(8,15),THGAIN
      COMMON /DERV/ BOLTZ(7,13),HFNU(7,13),FLUX,TAU(7,13),SIGNL(8)
      COMMON /RATES/ KFR(186),KBR(186),RCTF(186),RCTB(186),RF(186)
      COMMON /DILUENT/ SF6,AR,HE,N2
      COMMON /POWER/ PLINE(8,15),ELINE(8,15),PL
      COMMON /MISC/ LRATIO,JMAX(8)
      COMMON /BROAD/ CCC(126,10),GAMMA(8,15),PMOL(6),FB(15,8)
      COMMON /FLAME/ FLASH(2,20),Z1,Z2,PFLASH,WPHOTO
      COMMON /TITLE1/ RUNNUM
      COMMON /GAS1/ RH2,RF2,RF1,RO2,RHE,RN2,RSF6,RAR,PH1,RHF,PRESS,TEMP
      COMMON /CAVITY1/ R0,RL,LNTH,LSPOWER
      COMMON /IO/ TIMEL,TCHECK,POFF,ISKIP,IPEEK,KBS
      COMMON /INTEGR/ H,HMIN,HMAX,EPS,JSTART,KEY
      DIMENSION FBOLD(15,7)
      EQUIVALENCE (FB(1,1),FBOLD(1,1))
      REAL KFR,KBR,N2,LNTH,LRATIC
C
CC.....FOREIGN GAS LINE BROADENING PARAMETERS
C
      DATA FB/105*0.,.07,.07,.05,.06,.085,.085,.085,.085,.085,.085,.085,
     1.085,.085,.085,.085/
C
CC.....INPUT OF SPECTROSCOPIC AND THERMODYNAMIC DATA
CC.....ROTATIONAL ENERGY
C
      KEY=23
C
      READ (1,52) E
C
CC.....TRANSITION WAVE NUMBER, 1/CM
C
      READ (2,48) WC
C
CC.....EINSTEIN ISOTROPIC ABSORPTION COEFFICIENT
C
      READ (3,48) B
C
CC.....ROTATIONAL PARTITION FUNCTION
C
      READ (4,48) O
```


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```
      PROGRAM SPIKEHF                                                    12/21/77

C                                                                                SPIKEHF    55
C.....HEAT CAPACITY                                                              SPIKEHF    56
C                                                                                SPIKEHF    57
      READ(8,51) CVF,CVF2,CVN2,CVSF6,CVH2,CVHF,CVC,CVO2,CVOH,CVH2O,CVHO2         SPIKEHF    58
C                                                                                SPIKEHF    59
C.....ENTHALPY OF GASES                                                          SPIKEHF    60
C                                                                                SPIKEHF    61
      READ (9,49) EHPYF,EHPYF2,EHPYF,EHPYF2,EHPYHF,EHPYO,EHPYO2,EHPYCH,          SPIKEHF    62
     1 EHPYH2O,EHPYHO2                                                           SPIKEHF    63
C                                                                                SPIKEHF    64
C.....LINE WIDTH PARAMETERS.CCC ARE SELF-BROADENING COEFFICIENTS                 SPIKEHF    65
C.....OF MEREDITH, FB AND FBOLC ARE EXPERIMENTAL FOREIGN GAS                     SPIKEHF    66
C.....BROADENING LINE WIDTHS.  UNITS: 1/(CM-ATM)                                 SPIKEHF    67
      READ (14,53) CCC                                                           SPIKEHF    68
      READ (15,51) FBOLC                                                         SPIKEHF    69
      CALL INPUT1                                                                SPIKEHF    70
C                                                                                SPIKEHF    71
CC.....TRY REDUCING F2 BROADENING COEFFICIENT                                    SPIKEHF    72
CC                                                                               SPIKEHF    73
C                                                                                SPIKEHF    74
      F2RC=1.                                                                    SPIKEHF    75
      DO 1 J=1,15                                                                SPIKEHF    76
1     FB(J,3)=FB(J,3)/F2RC                                                       SPIKEHF    77
C                                                                                SPIKEHF    78
C.....CONVERTS GAS FRACTIONS TO MOLE/CC                                          SPIKEHF    79
C                                                                                SPIKEHF    80
      FCTR=.5348E-7*PRESS*(300./TEMP)                                            SPIKEHF    81
C                                                                                SPIKEHF    82
C.....INTEGRATION PARAMETERS FOR DIFSUB                                          SPIKEHF    83
C                                                                                SPIKEHF    84
      DELMIN=1.E-15                                                              SPIKEHF    85
      ALIM=DELMIN/100.                                                           SPIKEHF    86
      MAXDEP=8                                                                   SPIKEHF    87
      NEQN=150                                                                   SPIKEHF    88
      MF=0                                                                       SPIKEHF    89
      KKK=0                                                                      SPIKEHF    90
      TSTEP=TSKIP                                                                SPIKEHF    91
      NCT=0                                                                      SPIKEHF    92
C                                                                                SPIKEHF    93
C.....JCNT IS NC. STEPS BETWEEN. CHECK FOR J-SHIFTS                              SPIKEHF    94
C                                                                                SPIKEHF    95
      JCNT=1                                                                     SPIKEHF    96
      JGAIN=JCNT                                                                 SPIKEHF    97
C                                                                                SPIKEHF    98
C.....LASER POWER,PULSE ENERGY, ENERGY FOR EACH BAND                             SPIKEHF    99
C                                                                                SPIKEHF   100
      POWER=0.                                                                   SPIKEHF   101
      ENGY=0.                                                                    SPIKEHF   102
      PL=0.                                                                      SPIKEHF   103
      T=0.                                                                       SPIKEHF   104
      PFLASH=0.                                                                  SPIKEHF   105
      DO 2 I=1,8                                                                 SPIKEHF   106
      JMAX(I)=4                                                                  SPIKEHF   107
```


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```
      C
      C.....POWER,ENERGY,GAIN, FOR EACH LINE(TRANSITION), P(I,J)
      C
  110       DO 2 J=1,15
            PLINE(I,J)=0.
            ELINE(I,J)=0.
        2   ALPHA(I,J)=0.
            DO 3 I=1,NVAR
  115       Y(1,I)=0.
        3   YMAX(I)=1.E-6
      C
      C.....RCTF(I) IS FORWARD RATE OF REACT I,RCTB(I) IS BACKWARD
      C.....RATE OF REACT I, RF IS NET FORWARD RATE
  120 C
            DO 4 I=1,186
            RCTF(I)=0.
            RCTB(I)=0.
            RF(I)=0.
  125 C
      C.....DILUENT SPECIES CONCENTRATIONS, MOLES/CC
      C
            HE=RHE*FCTR
            N2=RN2*FCTR
  130       SF6=RSF6*FCTR
            AR=RAR*FCTR
      C
      C.....INITIAL VALUES  Y(1,N)                          N
      C.....HF(V) CONCENTRATION, V = N - 1                  1-9
  135 C.....UNDEFINED, RESERVED FOR ACO. VAR.               10-16
      C.....H-ATOM CONCENTRATION                            17
      C.....H2(V) CONCENTRATION  V = N - 18                 18-20
      C.....F-ATOM CONCENTRATION                            21
      C.....F2 CONCENTRATION                                22
  140 C.....TRANSLATIONAL TEMPERATURE                       23
      C.....PHOTON FLUX, F(V,N)                             24-79
      C
            Y(1,1)=RHF*FCTR
            Y(1,16)=RO2*FCTR
  145       Y(1,17)=RH1*FCTR
            Y(1,18)=RH2*FCTR
            Y(1,21)=RF1*FCTR
            Y(1,22)=RF2*FCTR
            Y(1,23)=TEMP
  150       DO 5 I=24,79
        5   Y(1,I)=FLUX
      C
      C.....CHECK TEMPERATURE AND READ CORRESPONDING
      C.....FORWARD(KFR) AND BACKWARD(KBR) RATE
  155 C.....COEFFICIENTS
      C
            AKT=(Y(1,23)-100.)/25.+1.5
            KT=IFIX(AKT)
            DO 5 I=1,KT
```

O_2

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```
      PROGRAM SPIKEHF                                                    12/21/77

      READ (12,50) KFR                                                  SPIKEHF  161
    5 READ (7,50) KBF                                                   SPIKEHF  162
      IF (N2.GT.0.) CALL RATE (Y(1,23))                                 SPIKEHF  163
      IF (SF6.GT.0.) CALL RATE (Y(1,23))                                SPIKEHF  164
      IF (BO2.GT.0.) CALL RATE (Y(1,23))                                SPIKEHF  165
C                                                                       SPIKEHF  166
C.....INTEGRATION LOOP                                                  SPIKEHF  167
C                                                                       SPIKEHF  168
      TOLD=T                                                            SPIKEHF  169
      IF (T.GT.TCHECK.AND.POWER.LT.PCOFF) TIMEL=T                       SPIKEHF  170
      IF (T1.EQ.0.) GO TO 10                                            SPIKEHF  171
C                                                                       SPIKEHF  172
C.....FLASHLAMP INTENSITY OBTAINED VIA INTERPOLATION                    SPIKEHF  173
C.....OF FLASHLAMP PROFILE                                              SPIKEHF  174
C                                                                       SPIKEHF  175
      KF=0                                                              SPIKEHF  176
      DO 9 I=1,20                                                       SPIKEHF  177
      TFL=FLASH(2,I)                                                    SPIKEHF  178
      IF (T.GE.TFL) KF=KF+1                                             SPIKEHF  179
      IF (T.LT.TFL) GO TO 8                                             SPIKEHF  180
    9 CONTINUE                                                          SPIKEHF  181
    8 PFLASH=FLASH(1,KF)+(T-FLASH(2,KF))*(FLASH(1,KF+1)-FLASH(1,KF))/(FL SPIKEHF  182
     1ASH(2,KF+1)-FLASH(2,KF))                                          SPIKEHF  183
      PFLASH=PFLASH*Z1*(1.-EXP(-Z2*Y(1,22)))                            SPIKEHF  184
   10 CONTINUE                                                          SPIKEHF  185
C                                                                       SPIKEHF  186
C.....CHECK TEMP. AND INPUT NEW RATE COEFFS. IF NEEDED.                 SPIKEHF  187
C                                                                       SPIKEHF  188
      AIKT=(Y(1,23)-100.)/25.+1.5                                       SPIKEHF  189
      IKT=IFIX(AIKT)                                                    SPIKEHF  190
      IF (KT.EQ.IKT) GO TO 13                                           SPIKEHF  191
      KTDIF=IKT-KT                                                      SPIKEHF  192
      IF (KTDIF.GT.0) GO TO 11                                          SPIKEHF  193
      PRINT 54                                                          SPIKEHF  194
      GO TO 47                                                          SPIKEHF  195
   11 KT=IKT                                                            SPIKEHF  196
      DO 12 I=1,KTDIF                                                   SPIKEHF  197
      READ (12,50) KFR                                                  SPIKEHF  198
   12 READ (7,50) KBF                                                   SPIKEHF  199
C                                                                       SPIKEHF  200
C.....COMPUTE RATE COEFFS. CORRESPONDING TO N2 OR                       SPIKEHF  201
C.....SF6 DEACTIVATION.                                                 SPIKEHF  202
C                                                                       SPIKEHF  203
      IF (N2.GT.0.) CALL RATE (Y(1,23))                                 SPIKEHF  204
      IF (SF6.GT.0.) CALL RATE (Y(1,23))                                SPIKEHF  205
      IF (BO2.GT.0.) CALL RATE (Y(1,23))                                SPIKEHF  206
C                                                                       SPIKEHF  207
C.....UPDATE SELF-BROADENED LINEWIDTH                                   SPIKEHF  208
C                                                                       SPIKEHF  209
   13 IF (T.EQ.0.) GO TO 500                                            SPIKEHF  210
      PMOL(1)=Y(1,1)                                                    SPIKEHF  211
      PMOL(2)=Y(1,2)                                                    SPIKEHF  212
      PMOL(3)=Y(1,3)+Y(1,4)+Y(1,5)+Y(1,6)+Y(1,7)+Y(1,8)+Y(1,9)          SPIKEHF  213
```

O_2

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```
      CALL LORENTZ (Y(1,23),15)                                          SPIKEHF  214
C                                                                        SPIKEHF  215
C.....CHECK FOR J-SHIFT IF NO. OF STEPS SINCE                            SPIKEHF  216
C.....LAST CHECK(JGAIN) IS .GE. JCNT                                     SPIKEHF  217
C                                                                        SPIKEHF  218
      JGAIN=JGAIN+1                                                      SPIKEHF  219
      IF (JGAIN-JCNT) 14,16,16                                           SPIKEHF  220
C                                                                        SPIKEHF  221
C.....COMPUTE GAIN FOR THE LINES NEAR J-MAX ONLY, THEN                   SPIKEHF  222
C.....PROCEED TO INTEGRATION                                             SPIKEHF  223
CC                                                                       SPIKEHF  224
C                                                                        SPIKEHF  225
14    DO 15 I=1,8                                                        SPIKEHF  226
      IV=I-1                                                             SPIKEHF  227
      JLOW=JMAX(I)-3                                                     SPIKEHF  228
      JHIGH=JMAX(I)+3                                                    SPIKEHF  229
      DO 15 J=JLOW,JHIGH                                                 SPIKEHF  230
15    ALPHA(I,J)=GAINC2(IV,J,79,Y)                                       SPIKEHF  231
      GO TO 29                                                           SPIKEHF  232
C                                                                        SPIKEHF  233
C.....COMPUTE GAIN FOR EACH POSSIBLE TRANSITION TO LOWER LEVEL (IV,J     SPIKEHF  234
C.....TO CHECK FOR J-SHIFT                                               SPIKEHF  235
C                                                                        SPIKEHF  236
16    JGAIN=0                                                            SPIKEHF  237
      DO 17 I=1,8                                                        SPIKEHF  238
      IV=I-1                                                             SPIKEHF  239
      DO 17 J=1,15                                                       SPIKEHF  240
17    ALPHA(I,J)=GAINC2(IV,J,79,Y)                                       SPIKEHF  241
C                                                                        SPIKEHF  242
C.....CHECK J-SHIFT                                                      SPIKEHF  243
C.....DETERMINE THE J    (LOWER LEVEL) OF MAX GAIN                       SPIKEHF  244
C                                                                        SPIKEHF  245
      DO 28 I=1,8                                                        SPIKEHF  246
      JMAXO=JMAX(I)                                                      SPIKEHF  247
      JMAX(I)=4                                                          SPIKEHF  248
      JM=4                                                               SPIKEHF  249
      DO 18 J=5,13                                                       SPIKEHF  250
      IF (ALPHA(I,J).LE.ALPHA(I,JM)) GO TO 18                            SPIKEHF  251
      JMAX(I)=J                                                          SPIKEHF  252
      JM=JMAX(I)                                                         SPIKEHF  253
18    CONTINUE                                                           SPIKEHF  254
      IF (JMAX(I).EQ.4) GO TO 19                                         SPIKEHF  255
      JMAX(I)=JMAX(I)-1                                                  SPIKEHF  256
19    CONTINUE                                                           SPIKEHF  257
      IF (JMAX(I).EQ.JMAXO) GO TO 28                                     SPIKEHF  258
C                                                                        SPIKEHF  259
C.....IF A J-SHIFT HAS OCCURRED, REDEFINE THE APPROPRIATE F(V,J) AND     SPIKEHF  260
C.....REINITIALIZE                                                       SPIKEHF  261
C.....THE Y(1,N) CORRESPONDING TO PHOTON FLUXES ARE                      SPIKEHF  262
C.....REDEFINED TO REPRESENT NEW TRANSITIONS IN EACH BAND                SPIKEHF  263
C                                                                        SPIKEHF  264
      JSTART=0                                                           SPIKEHF  265
      LJ=JMAX(I)-JMAXO                                                   SPIKEHF  266
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                L=7*I+16                                                        SPIKEHF   267
                IF (LJ.LT.0) GO TO 22                                           SPIKEHF   268
                IF (LJ.GE.7) GO TO 26                                           SPIKEHF   269
                KS=7-LJ                                                         SPIKEHF   270
      270       DO 20 M=1,KS                                                    SPIKEHF   271
           20   Y(1,L+M)=Y(1,L+LJ+M)                                            SPIKEHF   272
                DO 21 N=1,LJ                                                    SPIKEHF   273
           21   Y(1,L+N+KS)=FLUX                                                SPIKEHF   274
                GO TO 28                                                        SPIKEHF   275
      275       NLJ=-LJ                                                         SPIKEHF   276
           22   IF (NLJ.GE.7) GO TO 26                                          SPIKEHF   277
                NKS=7-NLJ                                                       SPIKEHF   278
                DO 23 M=1,NKS                                                   SPIKEHF   279
           23   STORE(M)=Y(1,L+M)                                               SPIKEHF   280
      280       DO 24 M=1,NKS                                                   SPIKEHF   281
           24   Y(1,L+NLJ+M)=STORE(M)                                           SPIKEHF   282
                DO 25 M=1,NLJ                                                   SPIKEHF   283
           25   Y(1,L+M)=FLUX                                                   SPIKEHF   284
                GO TO 28                                                        SPIKEHF   285
      285       DO 27 M=1,7                                                     SPIKEHF   286
           27   Y(1,L+M)=FLUX                                                   SPIKEHF   287
           28   CONTINUE                                                        SPIKEHF   288
C                                                                               SPIKEHF   289
C.........INTEGRATE                                                            SPIKEHF   290
C                                                                               SPIKEHF   291
      290       CALL DIFSUB (NVAR,T,Y,SAVE,H,HMIN,HMAX,EPS,MF,YMAX,ERROR,KFLAG,JST SPIKEHF   292
               1ART,MAXDER,PW,KEY)                                              SPIKEHF   293
                NCT=NCT+1                                                       SPIKEHF   294
                GO TO 31                                                        SPIKEHF   295
      295       C                                                               SPIKEHF   296
C.........RETRY LAST STEP WITH SMALLER STEP SIZE                                SPIKEHF   297
C                                                                               SPIKEHF   298
           30   H=HMIN                                                          SPIKEHF   299
                HMIN=HMIN/20.                                                   SPIKEHF   300
      300       JSTART=-1                                                       SPIKEHF   301
                GO TO 29                                                        SPIKEHF   302
           31   CONTINUE                                                        SPIKEHF   303
C                                                                               SPIKEHF   304
C.........IF INTEGRATION UNSUCCESSFUL, GO TO 45                                 SPIKEHF   305
      305       C                                                               SPIKEHF   306
                IF (KFLAG.LE.0) GO TO 45                                        SPIKEHF   307
C                                                                               SPIKEHF   308
C.........MAINTAIN MINIMUM PHOTON FLUXES AT "NOISE LEVEL"                       SPIKEHF   309
C                                                                               SPIKEHF   310
      310       DO 32 I=24,79                                                   SPIKEHF   311
                IF (Y(1,I).LT.FLUX) Y(1,I)=FLUX                                 SPIKEHF   312
           32   CONTINUE                                                        SPIKEHF   313
C                                                                               SPIKEHF   314
C.........COMPUTE LASER PULSE POWER(POWER) AND PULSE ENERGY(ENGY).              SPIKEHF   315
      315  C.........PLINE AND ELINE CORRESPOND TO POWER AND ENERGY FOR EACH      SPIKEHF   316
C.........TRANSITION.  H1 = STEP SIZE   CONST = CONVERSION FACTOR               SPIKEHF   317
C                                                                               SPIKEHF   318
                H1=T-TOLD                                                       SPIKEHF   319
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                CONST=2.85912*THGAIN                                                SPIKEHF   320
320             CONST=CONST*USPOWER                                                 SPIKEHF   321
                POWER=0.                                                            SPIKEHF   322
                DO 33 I=1,8                                                         SPIKEHF   323
                K=JMAX(I)-4                                                         SPIKEHF   324
                L=7*I+16                                                            SPIKEHF   325
325             DO 33 J=1,7                                                         SPIKEHF   326
                PLINE(I,K+J)=Y(1,L+J)**2*C(I,K+J)*CONST*4.184                       SPIKEHF   327
                POWER=POWER+PLINE(I,K+J)                                            SPIKEHF   328
          33    ELINE(I,K+J)=ELINE(I,K+J)+PLINE(I,K+J)*H1                           SPIKEHF   329
                ENGY=ENGY+POWER*H1                                                  SPIKEHF   330
330           C                                                                     SPIKEHF   331
              C.....CHECK FOR PULSE TERMINATION, PRINT STEP AND QUICK LOOK          SPIKEHF   332
              C.....OPTION(MINIMAL PRINT)                                           SPIKEHF   333
              C                                                                     SPIKEHF   334
                IF (T.GT.TIMEL) GO TO 500                                           SPIKEHF   335
335             IF (T.LE.TSTEP) GO TO 44                                            SPIKEHF   336
                TSTEP=TSTEP+TSKIP                                                   SPIKEHF   337
                IF (IPEEK.EQ.1) GO TO 41                                            SPIKEHF   338
              C                                                                     SPIKEHF   339
              C.....OUTPUT COMMANDS                                                 SPIKEHF   340
340           C                                                                     SPIKEHF   341
             500  CONTINUE                                                         SPIKEHF   342
                PRINT 499, RUNNUM                                                   SPIKEHF   343
            499   FORMAT(1H1,*RUN NO. SHF - *,I3,//)                                SPIKEHF   344
          34    PRINT 55, T,Y(1,23),NCT,H1                                          SPIKEHF   345
345             PRINT 56, POWER,ENGY                                                SPIKEHF   346
                PRINT 57                                                            SPIKEHF   347
                PRINT 58                                                            SPIKEHF   348
                PRINT 59, Y(1,17),Y(1,21),Y(1,22),Y(1,18),Y(1,19),Y(1,20)           SPIKEHF   349
                PRINT 60                                                            SPIKEHF   350
350             PRINT 61, (Y(1,I),I=1,9)                                            SPIKEHF   351
                PRINT 62                                                            SPIKEHF   352
                PRINT 61, Y(1,15),Y(1,16),(Y(1,I),I=80,83),N2,SF6                   SPIKEHF   353
                IF (K3S.LT.2) GO TO 41                                              SPIKEHF   354
                PRINT 63                                                            SPIKEHF   355
355             PRINT 64                                                            SPIKEHF   356
                DO 35 I=1,8                                                         SPIKEHF   357
                IV=I-1                                                              SPIKEHF   358
                L=7*I+16                                                            SPIKEHF   359
                PRINT 65, IV,JMAX(I),(Y(1,L+J),J=1,7)                               SPIKEHF   360
360       35    CONTINUE                                                          SPIKEHF   361
                PRINT 66                                                            SPIKEHF   362
                DO 36 I=1,8                                                         SPIKEHF   363
                IV=I-1                                                              SPIKEHF   364
                K=JMAX(I)-4                                                         SPIKEHF   365
365             PRINT 65, IV,JMAX(I),(ELINE(I,K+J),J=1,7)                           SPIKEHF   366
          36    CONTINUE                                                          SPIKEHF   367
                PRINT 67                                                            SPIKEHF   368
                PRINT 68                                                            SPIKEHF   369
                DO 37 J=1,15                                                        SPIKEHF   370
370             PRINT 71, J,(ELINE(I,J),I=1,8)                                      SPIKEHF   371
          37    CONTINUE                                                          SPIKEHF   372
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                IF (KBS.LT.3) GO TO 41                                          SPIKEHF   373
                PRINT 69                                                        SPIKEHF   374
                PRINT 70                                                        SPIKEHF   375
375             DO 38 J=1,15                                                    SPIKEHF   376
                PRINT 71, J,(ALPHA(I,J),I=1,8)                                  SPIKEHF   377
          38    CONTINUE                                                        SPIKEHF   378
                IF (KBS.LT.4) GO TO 41                                          SPIKEHF   379
                PRINT 72                                                        SPIKEHF   380
380             PRINT 69                                                        SPIKEHF   381
                DO 39 J=1,15                                                    SPIKEHF   382
                PRINT 71, J,(GAMMA(I,J),I=1,8)                                  SPIKEHF   383
          39    CONTINUE                                                        SPIKEHF   384
                IF (KBS.LT.5) GO TO 41                                          SPIKEHF   385
385             DO 40 J=1,4                                                     SPIKEHF   386
                PRINT 74                                                        SPIKEHF   387
                DO 40 I=1,50                                                    SPIKEHF   388
                K=(J-1)*50+I                                                    SPIKEHF   389
                IF (K.GT.186) GO TO 41                                          SPIKEHF   390
390             PRINT 73, K,KFR(K),KBR(K),RCTF(K),RCTB(K),RF(K)                 SPIKEHF   391
          40    CONTINUE                                                        SPIKEHF   392
          41    CONTINUE                                                        SPIKEHF   393
C                                                                               SPIKEHF   394
C.....WRITE OUTPUT TO TAPE 13                                                   SPIKEHF   395
395             DO 42 I=1,23                                                    SPIKEHF   396
          42    XXX(I)=Y(1,I)                                                   SPIKEHF   397
                XXX(24)=T                                                       SPIKEHF   398
                XXX(25)=POWER                                                   SPIKEHF   399
                XXX(26)=ENGY                                                    SPIKEHF   400
400             DO 43 I=1,8                                                     SPIKEHF   401
                DO 43 J=1,15                                                    SPIKEHF   402
                MVM=26+(I-1)*15+J                                               SPIKEHF   403
                NVN=146+(I-1)*15+J                                              SPIKEHF   404
                XXX(MVM)=PLINE(I,J)                                             SPIKEHF   405
405       43    XXX(NVN)=ALPHA(I,J)                                             SPIKEHF   406
                WRITE (13,48) XXX                                               SPIKEHF   407
                KKK=KKK+1                                                       SPIKEHF   408
C                                                                               SPIKEHF   409
C.....CHECK FOR TERMINATION. IF NOT, RETURN TO BEGINNING OF                     SPIKEHF   410
410 C.....INTEGRATION LOOP(7)                                                   SPIKEHF   411
C                                                                               SPIKEHF   412
                IF (T.EQ.0.) GO TO 29                                           SPIKEHF   413
          44    JSTART=1                                                        SPIKEHF   414
415             IF (T.LE.TIMEL) GO TO 7                                         SPIKEHF   415
                GO TO 46                                                        SPIKEHF   416
C                                                                               SPIKEHF   417
C.....INTEGRATION STEP WAS UNSUCCESSFUL. DETERMINE HERE WHETHER                 SPIKEHF   418
C.....TO TRY AGAIN WITH SMALLER STEP OR TO TERMINATE COMPUTATION.               SPIKEHF   419
C                                                                               SPIKEHF   420
420             IF (HMIN.GE.ALIM) GO TO 30                                      SPIKEHF   421
          45    PRINT 75, KFLAG,T                                               SPIKEHF   422
                CALL DIFFUN (T,Y,DERV1Y)                                        SPIKEHF   423
                PRINT 76, DERV1Y                                                SPIKEHF   424
                                                                                SPIKEHF   425
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      GO TO 47                                                                  SPIKEHF   426
C                                                                               SPIKEHF   427
C.....TERMINATION                                                               SPIKEHF   428
C                                                                               SPIKEHF   429
   46 PRINT 77, KKK                                                             SPIKEHF   430
   47 CONTINUE                                                                  SPIKEHF   431
C                                                                               SPIKEHF   432
   48 FORMAT (5E16.5)                                                           SPIKEHF   433
   49 FORMAT (5F16.5)                                                           SPIKEHF   434
   50 FORMAT (5E15.8)                                                           SPIKEHF   435
   51 FORMAT (5F16.5)                                                           SPIKEHF   436
   52 FORMAT (5E14.5)                                                           SPIKEHF   437
   53 FORMAT (7F10.5)                                                           SPIKEHF   438
   54 FORMAT (//5X,* TEMPERATURE HAS DROPPED*//)                                SPIKEHF   439
   55 FORMAT (* TIME=*,E11.5,* SEC,*,10X,*TEMPERATURE=*,E11.5,* K,*,10X,       SPIKEHF   440
     1*DIFSUB CALLED*,I6,* TIMES,*,10X,*STEP SIZE=*,E11.5,* SEC*)               SPIKEHF   441
   56 FORMAT (/* LASING POWER=*,E11.5,* WATTS/CC*,10X,* PULSE ENERGY=*,E       SPIKEHF   442
     111.5,* JOULES/CC*)                                                        SPIKEHF   443
   57 FORMAT (///* CONCENTRATIONS IN MOLES/CC*)                                SPIKEHF   444
   58 FORMAT (/11X,*H*,15X,*F*,14X,*F2*,12X,*H2(0)*,12X,*H2(1)*,12X,*H2(       SPIKEHF   445
     12)*)                                                                      SPIKEHF   446
   59 FORMAT (6E16.5)                                                           SPIKEHF   447
   60 FORMAT (//7X,*HF(0)*,10X,*HF(1)*,10X,*HF(2)*,10X,*HF(3)*,10X,*HF(4       SPIKEHF   448
     1)*,10X,*HF(5)*,10X,*HF(6)*,10X,*HF(7)*,10X,*HF(8)*)                      SPIKEHF   449
   61 FORMAT (9E15.5)                                                           SPIKEHF   450
   62 FORMAT (//10X,*O*,13X,*O2*,13X,*OH*,13X,*H2O*,12X,*FO2*,12X,*HO2*,       SPIKEHF   451
     112X,*N2*,13X,*SF6*)                                                       SPIKEHF   452
   63 FORMAT (///* PHOTON FLUX OF THE LASING LINES, IN MOLES/SEC/CM-SQUA       SPIKEHF   453
     1RE*)                                                                      SPIKEHF   454
   64 FORMAT (/4X,*V*,8X,*JMAX*,4X,*F(V,JMAX-3)*,5X,*F(V,JMAX-2)*,5X,*F(       SPIKEHF   455
     1V,JMAX-1)*,6X,*F(V,JMAX)*,6X,*F(V,JMAX+1)*,5X,*F(V,JMAX+2)*,5X,*F(       SPIKEHF   456
     2V,JMAX+3)*)                                                               SPIKEHF   457
   65 FORMAT (I5,I10,7E16.5)                                                    SPIKEHF   458
   66 FORMAT (///* POWER OF THE LASING TRANSITIONS, IN WATTS/CC*/)              SPIKEHF   459
   67 FORMAT (*1CONTRIBUTION TO PULSE ENERGY FROM EACH TRANSITION IN JOU        SPIKEHF   460
     1LES/CC*)                                                                  SPIKEHF   461
   68 FORMAT (/3X,*J*,8X,*HF(0,J)*,9X,*HF(1,J)*,9X,*HF(2,J)*,9X,*HF(3,J)       SPIKEHF   462
     1*,9X,*HF(4,J)*,9X,*HF(5,J)*,9X,*HF(6,J)*,9X,*HF(7,J)*)                    SPIKEHF   463
   69 FORMAT (///* THE GAIN FOR ALL POSSIBLE TRANSITIONS, IN 1/CM*)            SPIKEHF   464
   70 FORMAT (//3X,*J*,6X,*ALPHA(0,J)*,6X,*ALPHA(1,J)*,6X,*ALPHA(2,J)*,6       SPIKEHF   465
     1X,*ALPHA(3,J)*,6X,*ALPHA(4,J)*,6X,*ALPHA(5,J)*,6X,*ALPHA(6,J)*,6X,       SPIKEHF   466
     2*ALPHA(7,J)*)                                                             SPIKEHF   467
   71 FORMAT (I4,8E16.5)                                                        SPIKEHF   468
   72 FORMAT (*1HF SELF-BROADENING COEFFICIENTS,1/ATM-CM*)                      SPIKEHF   469
   73 FORMAT (I4,5E16.5)                                                        SPIKEHF   470
   74 FORMAT (#1#,3X,#K#,7X,#KBR(K)#,10X,#KBR(K)#,10X,#RCTF(K)#,9X,#RCTR       SPIKEHF   471
     1(K)#,8X,#RF(K)#/)                                                         SPIKEHF   472
   75 FORMAT (1X,*STEP UNSUCCESSFUL*//I5,E16.5)                                 SPIKEHF   473
   76 FORMAT (/1X,5E16.5)                                                       SPIKEHF   474
   77 FORMAT (1X,*UPPER LIMIT OF INTEGRATION REACHED,   KKK=*,I10)              SPIKEHF   475
      END                                                                       SPIKEHF   476
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      SUBROUTINE INPUT1                                                 SPIKEHF  477
      COMMON /NUMVAR/ NVAR,NSVAR,NFLAG,MFLAG,NEQN                       SPIKEHF  478
      COMMON /GAIN/ ALPHA(8,15),THGAIN                                  SPIKEHF  479
      COMMON /DEPV/ POLT7(7,13),HFVJ(7,13),FLUX,TAU(7,13),SIGNL(9)      SPIKEHF  480
      COMMON /MISC/ LRATIO,JMAX(8)                                      SPIKEHF  481
      COMMON /FLASH/ FLASH(2,20),Z1,Z2,PFLASH,WPHOTO                    SPIKEHF  482
      COMMON /TITLE1/ RUNNUM                                            SPIKEHF  483
      COMMON /GASES/ H2,F2,F,O2,HE,N2,SF6,AR,H,HF,PRESS,TEMP            SPIKEHF  484
      COMMON /CAVITY/ R0,RL,LATH,LSPCMR                                 SPIKEHF  485
      COMMON /IO/ TIMEL,TCHECK,PCPF,TSKIP,IPEEK,KBS                     SPIKEHF  486
      COMMON /INTEG/ DELTA,HMIN,HMAX,EPS,JSTART,KFV                     SPIKEHF  487
      REAL N2,LATH,LRATIO                                               SPIKEHF  488
      INTEGER RUNNUM                                                    SPIKEHF  489
      NAMELIST /TITLE/RUNNUM                                            SPIKEHF  490
      NAMELIST /GASES/ H2,F2,F,O2,HE,N2,SF6,AR,H,HF                     SPIKEHF  491
      NAMELIST /GAS/ PRESS,TEMP                                         SPIKEHF  492
      NAMELIST /CAVITY/ R0,RL,LATH,LRATIO,FLUX                          SPIKEHF  493
      NAMELIST /OUTPUT1/ TIMEL,TCHECK,PCPF,TSKIP,IPEEK,KBS              SPIKEHF  494
      NAMELIST /FLASH1/ Z1,Z2,WPHOTO                                    SPIKEHF  495
      NAMELIST /FLASH2/ FLASH                                           SPIKEHF  496
      NAMELIST /STEPS/ DELTA,HMIN,HMAX,EPS,JSTART,NVAR                  SPIKEHF  497
      READ(5,TITLE)                                                     SPIKEHF  498
      READ (5,SPECIES)                                                  SPIKEHF  499
      WRITE (6,SPECIES)                                                 SPIKEHF  500
      GASSUM=H2+F2+F+O2+HE+N2+SF6+AR+H+HF+F                             SPIKEHF  501
      H2=(H2/GASSUM)*100.                                               SPIKEHF  502
      F2=(F2/GASSUM)*100.                                               SPIKEHF  503
      F=(F/GASSUM)*100.                                                 SPIKEHF  504
      O2=(O2/GASSUM)*100.                                               SPIKEHF  505
      HE=(HE/GASSUM)*100.                                               SPIKEHF  506
      N2=(N2/GASSUM)*100.                                               SPIKEHF  507
      SF6=(SF6/GASSUM)*100.                                             SPIKEHF  508
      AR=(AR/GASSUM)*100.                                               SPIKEHF  509
      H=(H/GASSUM)*100.                                                 SPIKEHF  510
      HF=(HF/GASSUM)*100.                                               SPIKEHF  511
      READ (5,GAS)                                                      SPIKEHF  512
      WRITE (6,GAS)                                                     SPIKEHF  513
      READ (5,CAVITY)                                                   SPIKEHF  514
      WRITE (6,CAVITY)                                                  SPIKEHF  515
      READ (5,OUTPUT1)                                                  SPIKEHF  516
      WRITE (6,OUTPUT1)                                                 SPIKEHF  517
      READ (5,STEPS)                                                    SPIKEHF  518
      WRITE (6,STEPS)                                                   SPIKEHF  519
      READ (5,FLASH1)                                                   SPIKEHF  520
      IF (Z1.EQ.0..OR.Z2.EQ.0.) GO TO 2                                 SPIKEHF  521
C.....THE FOLLOWING STATEMENT MAY BE DIFFERENT ON DIFFERENT SYSTEMS     SPIKEHF  522
      IF (EOF(5)) 2,1                                                   SPIKEHF  523
    1 READ (5,FLASH2)                                                   SPIKEHF  524
      WRITE (6,FLASH1)                                                  SPIKEHF  525
      WRITE (6,FLASH2)                                                  SPIKEHF  526
      GO TO 3                                                           SPIKEHF  527
    2 Z1=0.                                                             SPIKEHF  528
    3 USPOWER=(1.-R0)/((1.+(R0/RL)**.5)*(1.-(R0*RL)**.5))               SPIKEHF  529
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      THGAIN=-ALOG(RO*RL)/(2.*LNTH)                                    SPIKEHF   530
      PRINT 99,RUNNUM                                                  SPIKEHF   531
   99 FORMAT(1H1/8H SPIKEHF,15(1H*),*SPIKEHF*,14(1H*),*   RUN NO. SHF - * SPIKEHF   532
     1,I3,3X,14(1H*),*SPIKEHF*,15(1H*),*SPIKEHF*)                      SPIKEHF   533
      PRINT 6                                                          SPIKEHF   534
      PRINT 7                                                          SPIKEHF   535
      PRINT 8, F,F2,H,H2,HE,AR,N2,HF,SF6,O2                            SPIKEHF   536
      H2=H2/100.                                                       SPIKEHF   537
      F2=F2/100.                                                       SPIKEHF   538
      F=F/100.                                                         SPIKEHF   539
      O2=O2/100.                                                       SPIKEHF   540
      HE=HE/100.                                                       SPIKEHF   541
      N2=N2/100.                                                       SPIKEHF   542
      SF6=SF6/100.                                                     SPIKEHF   543
      AR=AR/100.                                                       SPIKEHF   544
      H=H/100.                                                         SPIKEHF   545
      HF=HF/100.                                                       SPIKEHF   546
      PRINT 9                                                          SPIKEHF   547
      PRINT 10, PRESS,TEMP                                             SPIKEHF   548
      PRINT 11                                                         SPIKEHF   549
      PRINT 12                                                         SPIKEHF   550
      PRINT 13, RO,RL,LNTH,LRATIO,THGAIN,FLUX,USPOWER                  SPIKEHF   551
      PRINT 14                                                         SPIKEHF   552
      IF (Z1.EQ.0.) GO TO 4                                            SPIKEHF   553
      PRINT 15                                                         SPIKEHF   554
      PRINT 16                                                         SPIKEHF   555
      PRINT 17, Z1,Z2,WPHOTO,FLASH(1,1),FLASH(2,1)                     SPIKEHF   556
      PRINT 18, (FLASH(1,J),FLASH(2,J),J=2,20)                         SPIKEHF   557
      GO TO 5                                                          SPIKEHF   558
    4 PRINT 19                                                         SPIKEHF   559
    5 PRINT 20                                                         SPIKEHF   560
      PRINT 21, TIMEL,TCHECK,PCFF,TSKIP,IPEEK,KBS                      SPIKEHF   561
      PRINT 22                                                         SPIKEHF   562
      PRINT 23, DELTA,HMIN,HMAX,EPS,JSTART,NVAR                        SPIKEHF   563
      RETURN                                                           SPIKEHF   564
C                                                                      SPIKEHF   565
    6 FORMAT(//45X,*INITIAL CONDITIONS*///1X,*GAS MIXTURE (PERCENT)*/) SPIKEHF   566
    7 FORMAT (/8X,*F*,9X,*F2*,9X,*H*,10X,*H2*,9X,*HE*,9X,*AR*,9X,*N2*,9X SPIKEHF   567
     1,*HF*,8X,*SF6*,9X,*O2*)                                          SPIKEHF   568
    8 FORMAT (F11.4,F10.4,F12.4,F10.4,2F11.4,F12.4,F11.4,F10.4,F12.4)  SPIKEHF   569
    9 FORMAT (///1X,*GAS CONDITIONS*//5X,*PRESSURE (TORR)*,6X,*TEMPERATU SPIKEHF   570
     1RE (K)*)                                                         SPIKEHF   571
   10 FORMAT (F15.0,4X,F15.0)                                          SPIKEHF   572
   11 FORMAT (///1X,*OPTICAL CAVITY*//45X,*THRESHOLD*,8X,*FLUX*,10X,*AVA SPIKEHF   573
     1ILABLE*)                                                         SPIKEHF   574
   12 FORMAT (7X,*RO*,7X,*RL*,5X,*LNTH(CM)*,4X,*LRATIO*,4X,*GAIN(1/CM)*, SPIKEHF   575
  100 1X,*MOLE/CM2-SEC*,4X,*POWER FACTOR*)                             SPIKEHF   576
   13 FORMAT (2F9.3,F11.0,F10.0,F14.5,F14.1,F16.5)                     SPIKEHF   577
   14 FORMAT (///1X,*FLASHLAMP PARAMETERS*//)                          SPIKEHF   578
   15 FORMAT (22X,*WPHOTO*)                                            SPIKEHF   579
   16 FORMAT (6X,*Z1*,7X,*Z2*,5X,*(1/CM)*,9X,*I*,10X,*T(SEC)*)         SPIKEHF   580
  105 17 FORMAT (2F9.4,F8.1,5X,E10.3,4X,E10.3)                         SPIKEHF   581
   18 FORMAT (31X,E10.3,4X,E10.3)                                      SPIKEHF   582
   19 FORMAT (5X,*FLASHLAMP OPTION NOT USED*)                          SPIKEHF   583
   20 FORMAT (1H1///1X,*OUTPUT CONTROLS*//3X,*TIMEL(SEC)*,7X,*TCHECK(SEC SPIKEHF   584
     1)*,3X,*PCFF(W/CM3)*,3X,*TSKIP(SEC)*,3X,*IPEEK*,4X,*KBS*)         SPIKEHF   585
  110 21 FORMAT (E11.2,E13.1,2E14.1,2I8)                               SPIKEHF   586
   22 FORMAT (///1X,*INTEGRATION PARAMETERS*//5X,*H(SEC)*,4X,*HMIN(SEC)* SPIKEHF   587
     1,4X,*HMAX(SEC)*,5X,*EPS*,4X,*JSTART*,3X,*NVAR*)                  SPIKEHF   588
   23 FORMAT (2E11.1,F13.1,E11.1,I7,I8)                                SPIKEHF   589
      END                                                              SPIKEHF   590
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      FUNCTION GAINC2 (IV,J,A,Y)                                        SPIKEHF  591
C     THIS FUNCTION CALCULATES THE GAIN OF A P-BRANCH TRANSITION WITH   SPIKEHF  592
C     LOWER LEVEL HF(V,J)                                               SPIKEHF  593
C         THIS SUBROUTINE TO BE USED WITH PROGRAM MODELC2.              SPIKEHF  594
C                                                                       SPIKEHF  595
      DIMENSION Y(8,100)                                                SPIKEHF  596
      COMMON /DIFSUB/ YMAX(100),SAVE(12,100),ERROR(100),PW(10000)       SPIKEHF  597
      COMMON /SPECT/ E(10,31),WC(9,10),B(9,10),Q(9,61)                  SPIKEHF  598
      COMMON /CV/ CVM2(17),CVF(17),CVF2(17),CVHF(17),CVSFE(17),CVN2(17) SPIKEHF  599
      COMMON /CVOXG/ CVO(17),CVC2(17),CVOH(17),CVH2O(17),CVHO2(17)      SPIKEHF  600
      COMMON /EHPY/ EHPYM(17),EHPYF2(17),EHPYF(17),EHPYF2(17),EHPYHF(17) SPIKEHF  601
      COMMON /EHPYOXG/ EHPYO(17),EHPYO2(17),EHPYOH(17),EHPYH2O(17),EHPYH SPIKEHF  602
     102(17)                                                            SPIKEHF  603
      COMMON /NUMVAR/ NVAR,NRVAR,NFLAG,MFLAG,NEQN                       SPIKEHF  604
      COMMON /GAIN/ ALPHA(8,15),THGAIN                                  SPIKEHF  605
      COMMON /DERV/ BOLTZ(7,13),HFVJ(7,13),FLUX,TAU(7,13),SIGNL(8)      SPIKEHF  606
      COMMON /RATES/ KFR(186),KBR(186),RCTF(186),RCTB(186),RF(186)      SPIKEHF  607
      COMMON /DILUENT/ SF6,AR,HE,N2                                     SPIKEHF  608
      COMMON /POWER/ PLINE(8,15),ELINE(8,15),PL                         SPIKEHF  609
      COMMON /MISC/ LRATIO,JMAX(8)                                      SPIKEHF  610
      COMMON /BROAD/ BCC(126,10),GAMMA(8,15),PMOL(6),FB(15,8)           SPIKEHF  611
      REAL NUP,NON,N2,LONTZ                                             SPIKEHF  612
      TEM=Y(1,23)                                                       SPIKEHF  613
      AIT=TEM/100.+.5                                                   SPIKEHF  614
      IT=IFIX(AIT)                                                      SPIKEHF  615
C                                                                       SPIKEHF  616
C.....A ARE CONSTANTS USED IN ERROR FCN APPROXIMATION                   SPIKEHF  617
C                                                                       SPIKEHF  618
      A1=0.0705230784                                                   SPIKEHF  619
      A2=0.0422820123                                                   SPIKEHF  620
      A3=0.0092705272                                                   SPIKEHF  621
      A4=0.0001520143                                                   SPIKEHF  622
      A5=0.0002765672                                                   SPIKEHF  623
      A6=0.0000430638                                                   SPIKEHF  624
      WHF=20.01                                                         SPIKEHF  625
C                                                                       SPIKEHF  626
C.....DOPP AND LONTZ ARE DOPPLER AND LORENTZ LINEWIDTHS, RESPECT.       SPIKEHF  627
C                                                                       SPIKEHF  628
      DOPP=3.5811338E-7*WC(IV+1,J)*SQRT(TEM/WHF)                        SPIKEHF  629
C                                                                       SPIKEHF  630
C.....GAMMA= SELF-BROADENING COEFF. COMPUTED IN SUBROUTINE              SPIKEHF  631
C.....LORENTZ                                                           SPIKEHF  632
C                                                                       SPIKEHF  633
      H2SUM=Y(1,18)+Y(1,19)+Y(1,20)                                     SPIKEHF  634
      LONTZ=1421.27*SQRT(TEM)*((H2SUM+Y(1,16))*FB(J,1)+N2*FB(J,2)+Y(1,22 SPIKEHF  635
     1)*FB(J,3)+AR*FB(J,4)+HE*FB(J,5)+Y(1,17)*FB(J,6)+Y(1,21)*FB(J,7)+SF SPIKEHF  636
     26*FB(J,8))+(PMOL(1)+PMOL(2)+PMOL(3))*82.057*TEM*GAMMA(IV+1,J)     SPIKEHF  637
C                                                                       SPIKEHF  638
C.....COMPUTE VOIGT FUNCTION PER APPROX. OF ERROR FCN GIVEN             SPIKEHF  639
C.....IN ABRAMOWITZ AND STEGUN                                          SPIKEHF  640
C                                                                       SPIKEHF  641
      YLINE=0.83255461*LONTZ/DOPP                                       SPIKEHF  642
                                                                        SPIKEHF  643
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O_2

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      IF (YLINE.GT.(2.4)) GO TO 1                                       SPIKEHF   644
      PHI=(0.46971864/DOPP)*EXP(YLINE*YLINE)                            SPIKEHF   645
55    PHI=PHI*(1.+A1*YLINE+A2*YLINE**2+A3*YLINE**3+A4*YLINE**4+A5*YLINE* SPIKEHF   646
     1*5+A6*YLINE**6)**(-16)                                            SPIKEHF   647
      GO TO 2                                                           SPIKEHF   648
      CONST=2.*YLINE**2                                                 SPIKEHF   649
    1 PHI=(1.-CONST**(-1)+3.*CONST**(-2)-15.*CONST**(-3)+105.*CONST**(-4 SPIKEHF   650
60   1))/(3.14159265*LONTZ)                                             SPIKEHF   651
                                                                        SPIKEHF   652
C                                                                       SPIKEHF   653
C.....COMPUTE POPULATIONS IN UPPER(NUP) AND LOWER(NON) LEVELS,          SPIKEHF   654
C.....ASSUMING BOLTZMANN ROTATIONAL DISTRIBUTION.                       SPIKEHF   655
C                                                                       SPIKEHF   656
65    NUP=(Y(1,IV+2)*(2.*FLOAT(J)-1.)/Q(IV+2,IT+1))*EXP(-1.4387886*E(IV+ SPIKEHF   657
     12,J)/TEM)                                                         SPIKEHF   658
      NON=(Y(1,IV+1)*(2.*FLOAT(J)+1.)/Q(IV+1,IT+1))*EXP(-1.4387886*E(IV+ SPIKEHF   659
     11,J+1)/TEM)                                                       SPIKEHF   660
C                                                                       SPIKEHF   661
70  C.....COMPUTE GAIN                                                  SPIKEHF   662
C                                                                       SPIKEHF   663
      GAINC2=3.1753646E-11*WC(IV+1,J)*PHI*B(IV+1,J)*(((2.*FLOAT(J)+1.)/( SPIKEHF   664
     12.*FLOAT(J)-1.))*NUP-N(N)                                         SPIKEHF   665
75    RETURN                                                            SPIKEHF   666
      END
```


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SUBROUTINE LORENTZ                                                    12/21/77

      1               SUBROUTINE LORENTZ (T,M)                                  SPIKEHF   667
                      DIMENSION A(7), C(7,6,3), CC(126)                         SPIKEHF   668
                      REAL K2                                                   SPIKEHF   669
                      COMMON /BROAD/ CCC(126,10),GAMMA(8,15),PMOL(6),FB(15,8)   SPIKEHF   670
      5               EQUIVALENCE (CC(1),C(1,1,1))                              SPIKEHF   671
                C                                                               SPIKEHF   672
                C.....THIS SUBROUTINE COMPUTES SELF-BROADENING COEFF. GAMMA     SPIKEHF   673
                C.....FOR BOTH HF AND DF MODELS.                                SPIKEHF   674
                C.....CCC(126,10) REFERS TO THE 126 COEFFICIENTS USED FOR EACH  SPIKEHF   675
     10         C.....OF 10 BANDS, 5HF AND 5 DF: HF(0-1),...,HF(4-5), DF(0-1),..SPIKEHF   676
                C.....,DF(4-5)                                                  SPIKEHF   677
                C.....CC(126) REPRESENTS SUCCESSIVELY THE 126 ELEMENTS IN EACH  SPIKEHF   678
                C.....OF THE BANDS, AS THE DO-LOOP PROGRESSES                   SPIKEHF   679
                C.....C(7,6,3) SORTS CC INTO GROUPS OF 7 COEFFICIENTS, USED TO  SPIKEHF   680
     15         C.....COMPUTE BROADENING BY EACH OF 6 SPECIES, AT 3 TEMPERATURES SPIKEHF   681
                C.....KT IS USED TO INTERPOLATE/EXTRAPOLATE BETWEEN TEMPERATURES SPIKEHF   682
                C.....GAMMA= SELF-BROADENING COEFFICIENT, 1/CM-ATM               SPIKEHF   683
                C                                                               SPIKEHF   684
                      KT=IFIX(T/300.)                                           SPIKEHF   685
     20               IF (T.LE.300.) KT=1                                       SPIKEHF   686
                      IF (T.GE.900.) KT=2                                       SPIKEHF   687
                C                                                               SPIKEHF   688
                C.....PMOLSUM = TOTAL HF AND DF POPULATION                      SPIKEHF   689
                C.....PMOL(1) = HF(0)                                           SPIKEHF   690
     25         C.....PMOL(2) = HF(1)                                           SPIKEHF   691
                C.....PMOL(3) = HF(2,...9)                                      SPIKEHF   692
                C.....PMOL(4) = DF(0)                                           SPIKEHF   693
                C.....PMOL(5) = DF(1)                                           SPIKEHF   694
                C.....PMOL(6) = DF(2,...10)                                     SPIKEHF   695
     30         C                                                               SPIKEHF   696
                      PMOLSUM=PMOL(1)+PMOL(2)+PMOL(3)+PMOL(4)+PMOL(5)+PMOL(6)   SPIKEHF   697
                      IF (PMOLSUM.LE.0.) GO TO 5                                SPIKEHF   698
                      DO 3 IV=1,5                                               SPIKEHF   699
                      DO 1 I=1,126                                              SPIKEHF   700
     35         1     CC(I)=CCC(I,IV)                                           SPIKEHF   701
                      DO 2 I=1,7                                                SPIKEHF   702
                      A(I)=0.                                                   SPIKEHF   703
                      DO 2 J=1,6                                                SPIKEHF   704
                      CI=C(I,J,KT)+(C(I,J,KT+1)-C(I,J,KT))*(T-300.*KT)/300.     SPIKEHF   705
     40         2     A(I)=A(I)+CI*PMOL(J)/PMOLSUM                              SPIKEHF   706
                      DO 3 K=1,M                                                SPIKEHF   707
                      K2=K*K                                                    SPIKEHF   708
                3     GAMMA(IV,K)=A(1)+A(2)*EXP(-K/4.)+A(3)*K*EXP(-K/4.)+A(4)*K2*EXP(-K/SPIKEHF   709
                     12.)+A(5)*K*EXP(-K2/8.)+A(6)*K2*EXP(-K2/16.)+A(7)*EXP(-K2/8.)  SPIKEHF   710
     45               DO 4 I=1,3                                                SPIKEHF   711
                      II=I+5                                                    SPIKEHF   712
                      DO 4 K=1,M                                                SPIKEHF   713
                4     GAMMA(II,K)=GAMMA(5,K)                                    SPIKEHF   714
                      GO TO 7                                                   SPIKEHF   715
     50         5     DO 6 I=1,8                                                SPIKEHF   716
                      DO 6 J=1,15                                               SPIKEHF   717
                6     GAMMA(I,J)=0.                                             SPIKEHF   718
                7     CONTINUE                                                  SPIKEHF   719
                      RETURN                                                    SPIKEHF   720
     55               END                                                       SPIKEHF   721
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      SUBROUTINE DIFFUN (T,Y,DERV1Y,KFLAG)                                  SPIKEHF  722
C                                                                           SPIKEHF  723
C THIS SUBROUTINE TO BE USED WITH MODELC                                    SPIKEHF  724
C                                                                           SPIKEHF  725
      DIMENSION Y(8,100), DERV1Y(100), VVHF(8), VTHF(8), VTH2(8), SEM(8)    SPIKEHF  726
      COMMON /DIFSUB/ YMAX(100),SAVE(12,100),ERROR(100),PW(10000)           SPIKEHF  727
      COMMON /SPECT/ E(10,31),WC(9,18),B(9,18),Q(9,61)                      SPIKEHF  728
      COMMON /CV/ CVH2(17),CVF(17),CVF2(17),CVHF(17),CVSFE(17),CVN2(17)     SPIKEHF  729
      COMMON /CVOXG/ CVO(17),CVO2(17),CVOH(17),CVH2O(17),CVHO2(17)          SPIKEHF  730
      COMMON /EHPY/ EHPYH(17),EHPYH2(17),EHPYF(17),EHPYF2(17),EHPYHF(17)    SPIKEHF  731
      COMMON /EHPYCXG/ EHPYC(17),EHPYC2(17),EHPYOH(17),EHPYH2O(17),EHPYH     SPIKEHF  732
     1O2(17)                                                                SPIKEHF  733
      COMMON /NUMVAR/ NVAR,NFVAR,NFLAG,MFLAG,NEQN                           SPIKEHF  734
      COMMON /GAIN/ ALPHA(8,15),THGAIN                                      SPIKEHF  735
      COMMON /DERV/ EOLTZ(7,13),FVJ(7,13),FLUX,TAU(7,13),SIGNL(8)           SPIKEHF  736
      COMMON /RATES/ KFR(186),KBR(186),RCTF(186),RCTB(186),RF(186)          SPIKEHF  737
      COMMON /DILUENT/ SF6,AR,HE,N2                                         SPIKEHF  738
      COMMON /POWER/ PLINE(8,15),ELINE(8,15),PL                             SPIKEHF  739
      COMMON /MISC/ LRATIO,JMAX(8)                                          SPIKEHF  740
      COMMON /FLAMP/ FLASH(2,20),Z1,Z2,PFLASH,WPHOTO                        SPIKEHF  741
      REAL M1,M2,M3,M4,M5,M6,M7,M8,M9,M10,KFR,KBR,N2,M11,LRATIO             SPIKEHF  742
      REAL M12,M13,M14,M15,M16                                              SPIKEHF  743
C                                                                           SPIKEHF  744
C.........DEFINE CATALYTIC SPECIES                                         SPIKEHF  745
C                                                                           SPIKEHF  746
      M5=Y(1,1)                                                             SPIKEHF  747
      DO 1 I=2,9                                                            SPIKEHF  748
    1 M5=M5+Y(1,I)                                                          SPIKEHF  749
      M4=Y(1,17)                                                            SPIKEHF  750
      M9=Y(1,18)+Y(1,19)+Y(1,20)                                            SPIKEHF  751
      M16=Y(1,15)+Y(1,16)+Y(1,80)+Y(1,81)+Y(1,82)+Y(1,83)                   SPIKEHF  752
      FSUM=Y(1,21)+Y(1,22)                                                  SPIKEHF  753
      HEARF=HE+AR+FSUM                                                      SPIKEHF  754
      M1=M5+2.4*FSUM+HE+AR+M9+M4                                            SPIKEHF  755
      M2=M5+HEARF+2.5*M9+20.*M4+N2                                          SPIKEHF  756
      M11=N2+SF6+0.3*Y(1,16)                                  <-O2          SPIKEHF  757
      M3=M5+HEARF+M9+M4+M11+M16                                             SPIKEHF  758
      M6=Y(1,21)                                                            SPIKEHF  759
      M7=Y(1,22)+AR                                                         SPIKEHF  760
      M8=HE                                                                 SPIKEHF  761
      M10=HEARF+4.*M9+4.*M4+N2+M5                                           SPIKEHF  762
      M12=2.82*Y(1,15)+Y(1,16)                                              SPIKEHF  763
      M13=N2                                                                SPIKEHF  764
      M14=M3+Y(1,16)+1.8*(M9+Y(1,81))                                       SPIKEHF  765
      M15=M3+5.1*Y(1,81)                                                    SPIKEHF  766
C                                                                           SPIKEHF  767
C THE FOLLOWING ARE THE COLD PUMPING REACTIONS                              SPIKEHF  768
C                                                                           SPIKEHF  769
      DO 2 I=1,6                                                            SPIKEHF  770
      RCTF(10+I)=Y(1,18)*Y(1,21)*KFR(10+I)                                  SPIKEHF  771
    2 RCTB(10+I)=Y(1,17)*Y(1,10+I)*KBR(10+I)                                SPIKEHF  772
C                                                                           SPIKEHF  773
C THE FOLLOWING ARE THE HOT PUMPING REACTIONS                               SPIKEHF  774
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C                                                                       SPIKEHF   775
      DO 3 I=1,9                                                        SPIKEHF   776
      RCTF(16+I)=Y(1,17)*Y(1,22)*KFR(16+I)                              SPIKEHF   777
    3 RCTB(16+I)=Y(1,21)*Y(1,I)*KBR(16+I)                               SPIKEHF   778
C                                                                       SPIKEHF   779
CC THE FOLLOWING ARE THE V-T DEACTIVATION REACTIONS                     SPIKEHF   780
C                                                                       SPIKEHF   781
      DO 4 I=1,8                                                        SPIKEHF   782
      RCTF(25+I)=M5*Y(1,I+1)*KFR(25+I)                                  SPIKEHF   783
      RCTB(25+I)=M5*Y(1,I)*KBR(25+I)                                    SPIKEHF   784
      RCTF(33+I)=M5*Y(1,I+1)*KFR(33+I)                                  SPIKEHF   785
      RCTB(33+I)=M5*Y(1,I)*KBR(33+I)                                    SPIKEHF   786
      RCTF(41+I)=M6*Y(1,I+1)*KFR(41+I)                                  SPIKEHF   787
      RCTB(41+I)=M6*Y(1,I)*KBR(41+I)                                    SPIKEHF   788
      RCTF(49+I)=M7*Y(1,I+1)*KFR(49+I)                                  SPIKEHF   789
      RCTB(49+I)=M7*Y(1,I)*KBR(49+I)                                    SPIKEHF   790
      RCTF(93+I)=M8*Y(1,I+1)*KFR(93+I)                                  SPIKEHF   791
      RCTB(93+I)=M8*Y(1,I)*KBR(93+I)                                    SPIKEHF   792
      RCTF(101+I)=M9*Y(1,I+1)*KFR(101+I)                                SPIKEHF   793
      RCTB(101+I)=M9*Y(1,I)*KBR(101+I)                                  SPIKEHF   794
C                                                                       SPIKEHF   795
CC THE FOLLOWING ARE MULTI-QUANTA V-T DEACTIVATIONS                     SPIKEHF   796
C                                                                       SPIKEHF   797
      RCTF(57+I)=M4*Y(1,3)*KFR(57+I)                                    SPIKEHF   798
    4 RCTB(57+I)=M4*Y(1,9-I)*KBR(57+I)                                  SPIKEHF   799
      DO 5 I=1,7                                                        SPIKEHF   800
      RCTF(65+I)=M4*Y(1,8)*KFR(65+I)                                    SPIKEHF   801
    5 RCTB(65+I)=M4*Y(1,8-I)*KBR(65+I)                                  SPIKEHF   802
      DO 6 I=1,6                                                        SPIKEHF   803
      RCTF(72+I)=M4*Y(1,7)*KFR(72+I)                                    SPIKEHF   804
    6 RCTB(72+I)=M4*Y(1,7-I)*KBR(72+I)                                  SPIKEHF   805
      DO 7 I=1,5                                                        SPIKEHF   806
      RCTF(78+I)=M4*Y(1,6)*KFR(78+I)                                    SPIKEHF   807
    7 RCTB(78+I)=M4*Y(1,6-I)*KBR(78+I)                                  SPIKEHF   808
      DO 8 I=1,4                                                        SPIKEHF   809
      RCTF(83+I)=M4*Y(1,5)*KFR(83+I)                                    SPIKEHF   810
    8 RCTB(83+I)=M4*Y(1,5-I)*KBR(83+I)                                  SPIKEHF   811
      DO 9 I=1,3                                                        SPIKEHF   812
      RCTF(87+I)=M4*Y(1,4)*KFR(87+I)                                    SPIKEHF   813
    9 RCTB(87+I)=M4*Y(1,4-I)*KBR(87+I)                                  SPIKEHF   814
      DO 10 I=1,2                                                       SPIKEHF   815
      RCTF(90+I)=M4*Y(1,3)*KFR(90+I)                                    SPIKEHF   816
   10 RCTB(90+I)=M4*Y(1,3-I)*KBR(90+I)                                  SPIKEHF   817
      RCTF(93)=M4*Y(1,2)*KFR(93)                                        SPIKEHF   818
      RCTB(93)=M4*Y(1,1)*KBR(93)                                        SPIKEHF   819
C                                                                       SPIKEHF   820
CC THE FOLLOWING ARE HF-HF V-V EXCHANGE REACTIONS(NEGLECT 117,124,130)  SPIKEHF   821
C                                                                       SPIKEHF   822
      DO 11 I=1,7                                                       SPIKEHF   823
      RCTF(109+I)=Y(1,I+1)*Y(1,I+1)*KFR(109+I)                          SPIKEHF   824
   11 RCTB(109+I)=Y(1,I)*Y(1,I+2)*KBR(109+I)                            SPIKEHF   825
      DO 12 I=1,6                                                       SPIKEHF   826
      RCTF(117+I)=Y(1,I+1)*Y(1,I+2)*KFR(117+I)                          SPIKEHF   827
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                12    RCTB(117+I)=Y(1,I)*Y(1,I+3)*KBR(117+I)
                      DO 13 I=1,5
                      RCTF(124+I)=Y(1,I+1)*Y(1,I+3)*KFR(124+I)
110             13    RCTB(124+I)=Y(1,I)*Y(1,I+4)*KBR(124+I)
                      DO 14 I=1,4
                      RCTF(130+I)=Y(1,I+1)*Y(1,I+4)*KFR(130+I)
                      RCTB(130+I)=Y(1,I)*Y(1,I+5)*KBR(130+I)
                C
115             CCC THE FOLLOWING ARE HF-H2 V-V EXCHANGE REACTIONS
                C
                      RCTF(134+I)=Y(1,I)*Y(1,19)*KFR(134+I)
                14    RCTB(134+I)=Y(1,I+1)*Y(1,18)*KBR(134+I)
                      DO 15 I=1,2
120                   RCTF(138+I)=Y(1,I)*Y(1,20)*KFR(138+I)
                      RCTB(138+I)=Y(1,I+1)*Y(1,19)*KBR(138+I)
                C
                CCC THE FOLLOWING ARE V-T DEACTIVATIONS FOR H2(V)
                CCC
125                   RCTF(140+I)=M10*Y(1,18+I)*KFR(140+I)
                15    RCTB(140+I)=M10*Y(1,17+I)*KBR(140+I)
                      DO 16 I=1,8
                      RCTF(142+I)=Y(1,I+1)*M11*KFR(142+I)
                16    RCTB(142+I)=Y(1,I)*M11*KBR(142+I)
130                   RCTF(151)=Y(1,15)*Y(1,15)*M12*KFR(151)
                      RCTB(151)=Y(1,16)*M12*KBR(151)
                      RCTF(152)=Y(1,15)*Y(1,15)*M13*KFR(152)
                      RCTB(152)=Y(1,16)*M13*KBR(152)
                      RCTF(153)=Y(1,18)*Y(1,80)*KFR(153)
135                   RCTB(153)=Y(1,17)*Y(1,81)*KBR(153)
                      RCTF(154)=Y(1,17)*Y(1,16)*KFR(154)
                      RCTB(154)=Y(1,15)*Y(1,80)*KBR(154)
                      RCTF(155)=Y(1,15)*Y(1,18)*KFR(155)
                      RCTB(155)=Y(1,17)*Y(1,80)*KBR(155)
140                   RCTF(156)=Y(1,17)*Y(1,16)*M14*KFR(156)
                      RCTB(156)=Y(1,83)*M14*KBR(156)
                      RCTF(157)=Y(1,17)*Y(1,80)*M15*KFR(157)
                      RCTB(157)=Y(1,81)*M15*KBR(157)
                      RCTF(158)=Y(1,17)*Y(1,15)*M3*KFR(158)
145                   RCTB(158)=Y(1,80)*M3*KBR(158)
                      RCTF(159)=Y(1,15)*Y(1,82)*M3*KFR(159)
                      RCTB(159)=Y(1,83)*M3*KBR(159)
                      RCTF(160)=Y(1,15)*Y(1,81)*KFR(160)
                      RCTB(160)=Y(1,80)*Y(1,80)*KBR(160)
150                   RCTF(161)=Y(1,17)*Y(1,83)*KFR(161)
                      RCTB(161)=Y(1,80)*Y(1,80)*KBR(161)
                      RCTF(162)=Y(1,17)*Y(1,83)*KFR(162)
                      RCTB(162)=Y(1,16)*Y(1,18)*KBR(162)
                      RCTF(163)=Y(1,15)*Y(1,83)*KFR(163)
155                   RCTB(163)=Y(1,16)*Y(1,80)*KBR(163)
                      RCTF(164)=Y(1,16)*Y(1,21)*M3*KFR(164)
                      RCTB(164)=Y(1,82)*M3*KBR(164)
                      DO 17 I=11,NEQN
                17    RF(I)=RCTF(I)-RCTB(I)
```

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SPIKEHF 828 through SPIKEHF 879

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```
C
C  VTHF(I) IS THE V-T DEACTIVATION RATE OF HF FROM HF(I) TO HF(I-1)
C
      DO 18 I=1,8
18    VTHF(I)=RF(25+I)+RF(33+I)+RF(41+I)+RF(49+I)+RF(93+I)+RF(101+I)
C
C  VTH2(I) IS THE V-T DEACTIVATION RATE OF H2 FROM H2(I) TO H2(I-1)
C
      VTH2(1)=RF(135)+RF(136)+RF(137)+RF(138)+RF(141)
      VTH2(2)=RF(139)+RF(140)+RF(142)
C
C  THE PUMPING TERMS SUMMED
C
      COLD=RF(11)+RF(12)+RF(13)+RF(14)+RF(15)+RF(16)
      HOT=RF(17)+RF(18)+RF(19)+RF(20)+RF(21)+RF(22)+RF(23)+RF(24)+RF(25)
C
C  VVHF(I) ARE SOME V-V EXCHANGE TERMS FOR HF-HF.  ADD TO HF(I-1) TERM
C
      VVHF(1)=RF(118)+RF(125)+RF(131)-RF(135)-RF(139)
      VVHF(2)=RF(119)+RF(126)+RF(132)-RF(136)-RF(140)
      VVHF(3)=-RF(118)+RF(120)+RF(127)+RF(133)-RF(137)
      VVHF(4)=-RF(119)+RF(121)-RF(125)+RF(128)+RF(134)-RF(138)
      VVHF(6)=-RF(121)+RF(123)-RF(127)-RF(132)
      VVHF(5)=-RF(120)+RF(122)-RF(126)+RF(129)-RF(131)
      VVHF(7)=-RF(122)-RF(128)-RF(133)
      VVHF(8)=-RF(123)-RF(129)-RF(134)
      DO 19 I=1,NVAR
19    DERV1Y(I)=0.
C
C  TIME DERIVATIVE OF THE CONCENTRATIONS DUE TO CHEMISTRY ONLY
C
      DERV1Y(1)=RF(17)+RF(65)+RF(72)+RF(78)+RF(83)+RF(87)+RF(90)+RF(92)+
     1RF(93)+RF(110)+VTHF(1)+VVHF(1)
      DERV1Y(2)=RF(11)+RF(18)+RF(64)+RF(71)+RF(77)+RF(82)+RF(86)+RF(89)+
     1RF(91)-RF(93)-2.*RF(110)+RF(111)-VTHF(1)+VTHF(2)-VVHF(1)+VVHF(2)
      DERV1Y(3)=RF(12)+RF(19)+RF(63)+RF(70)+RF(76)+RF(81)+RF(85)+RF(88)-
     1RF(91)-RF(92)+RF(110)-2.*RF(111)+RF(112)-VTHF(2)+VTHF(3)-VVHF(2)+V
     2VHF(3)
      DERV1Y(4)=RF(13)+RF(20)+RF(62)+RF(69)+RF(75)+RF(80)+RF(84)-RF(88)-
     1RF(89)-RF(90)+RF(111)-2.*RF(112)+RF(113)+VTHF(4)-VTHF(3)+VVHF(4)-V
     2VHF(3)
      DERV1Y(5)=RF(14)+RF(21)+RF(61)+RF(68)+RF(74)+RF(79)-RF(84)-RF(85)-
     1RF(86)-RF(87)+RF(112)-2.*RF(113)+RF(114)+VTHF(5)-VTHF(4)+VVHF(5)-V
     2VHF(4)
      DERV1Y(6)=RF(15)+RF(22)+RF(61)+RF(67)+RF(73)-RF(79)-RF(80)-RF(81)-
     1RF(82)-RF(83)+RF(113)-2.*RF(114)+RF(115)+VTHF(6)-VTHF(5)+VVHF(6)-V
     2VHF(5)
      DERV1Y(7)=RF(16)+RF(23)+RF(59)+RF(66)-RF(73)-RF(74)-RF(75)-RF(76)-
     1RF(77)-RF(78)+RF(114)-2.*RF(115)+RF(116)+VTHF(7)-VTHF(6)+VVHF(7)-V
     2VHF(6)
      DERV1Y(8)=RF(24)+RF(58)-RF(66)-RF(67)-RF(68)-RF(69)-RF(70)-RF(71)-
     1RF(72)+RF(115)-2.*RF(116)+VTHF(8)-VTHF(7)+VVHF(8)-VVHF(7)
      DERV1Y(9)=RF(25)-RF(58)-RF(59)-RF(60)-RF(61)-RF(62)-RF(63)-RF(64)-
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SPIKEHF 881 through SPIKEHF 937

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```
     1RF(65)+RF(116)-VTHF(8)-VVHF(8)                                    SPIKEHF   934
C                                                                       SPIKEHF   935
C.....N2 V-T DEACTIVATION REACTIONS                                     SPIKEHF   936
C                                                                       SPIKEHF   937
      DERV1Y(1)=DERV1Y(1)+RF(143)                                       SPIKEHF   938
      DERV1Y(9)=DERV1Y(9)-RF(150)                                       SPIKEHF   939
      DO 20 I=2,8                                                       SPIKEHF   940
20    DERV1Y(I)=DERV1Y(I)+RF(142+I)-RF(141+I)                           SPIKEHF   941
C                                                                       SPIKEHF   942
C   NOW ADD MULTI-QUANTA (DELTA V .GT.1) DEACTIVATION BY HF             SPIKEHF   943
C                                                                       SPIKEHF   944
      RCTFMQ=0.                                                         SPIKEHF   945
      DO 21 I=1,9                                                       SPIKEHF   946
      FK=8.-FLOAT(I)                                                    SPIKEHF   947
      IF (I.GT.8) FK=0.                                                 SPIKEHF   948
      F2=1.                                                             SPIKEHF   949
      IF (I.LE.2) F2=0.                                                 SPIKEHF   950
      RCTFMQ=RCTFMQ+F2*(RCTF(36-I)+RCTF(44-I))                          SPIKEHF   951
21    DERV1Y(10-I)=DERV1Y(10-I)+RCTFMQ-FK*(RCTF(34-I)+RCTF(42-I))       SPIKEHF   952
      DO 22 I=10,16                                                     SPIKEHF   953
22    DERV1Y(I)=0.                                                      SPIKEHF   954
      DERV1Y(17)=COLD-HOT                                               SPIKEHF   955
      DERV1Y(18)=VTH2(1)-COLD                                           SPIKEHF   956
      DERV1Y(19)=VTH2(2)-VTH2(1)                                        SPIKEHF   957
      DERV1Y(20)=-VTH2(2)                                               SPIKEHF   958
C                                                                       SPIKEHF   959
C.....EFFECT OF FLASHLAMP ON F AND F2 CONCENTRATIONS.                   SPIKEHF   960
C                                                                       SPIKEHF   961
      DERV1Y(21)=-DERV1Y(17)+2.*FFLASH                                  SPIKEHF   962
      DERV1Y(22)=-HOT-PFLASH                                            SPIKEHF   963
      PPHOTO=2.85912*WPHOTO*FFLASH                                      SPIKEHF   964
C                                                                       SPIKEHF   965
C.....OXYGEN KINETICS                                                   SPIKEHF   966
C                                                                       SPIKEHF   967
      DERV1Y(15)=DERV1Y(15)-2.*(RF(151)+RF(152))+RF(154)-RF(155)-RF(158)  SPIKEHF   968
     1-RF(159)-RF(160)-RF(163)                                          SPIKEHF   969
      DERV1Y(16)=DERV1Y(16)+RF(151)+RF(152)-RF(154)-RF(156)+RF(162)+RF(1  SPIKEHF   970
     163)-RF(164)                                                       SPIKEHF   971
      DERV1Y(17)=DERV1Y(17)+RF(153)-RF(154)+RF(155)-RF(156)-RF(157)-RF(1  SPIKEHF   972
     158)-RF(161)-RF(162)                                               SPIKEHF   973
      DERV1Y(18)=DERV1Y(18)-RF(153)-RF(155)+RF(162)                     SPIKEHF   974
      DERV1Y(21)=DERV1Y(21)-RF(164)                                     SPIKEHF   975
      DERV1Y(80)=DERV1Y(80)-RF(153)+RF(154)+RF(155)-RF(157)+RF(158)-RF(1  SPIKEHF   976
     159)+2.*(RF(160)+RF(161))+RF(163)                                  SPIKEHF   977
      DERV1Y(81)=DERV1Y(81)+RF(153)+RF(157)-RF(160)                     SPIKEHF   978
      DERV1Y(82)=DERV1Y(82)+RF(164)                                     SPIKEHF   979
      DERV1Y(83)=DERV1Y(83)+RF(156)+RF(159)-RF(161)-RF(162)-RF(163)     SPIKEHF   980
C                                                                       SPIKEHF   981
C EFFECT OF RADIATION ON HF(V) CONCENTRATION                            SPIKEHF   982
C     SIGNL(I) IS TOTAL RATE OF EMISSION FROM HF(I) TO HF(I-1)          SPIKEHF   983
C                                                                       SPIKEHF   984
      DO 23 I=1,8                                                       SPIKEHF   985
      L=7*I+16                                                          SPIKEHF   986
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```
      SUBROUTINE DIFFUN                                                  12/21/77

            K=JMAX(I)-4                                                                SPIKEHF    987
         23 SIGNL(I)=ALPHA(I,K+1)*Y(1,L+1)+ALPHA(I,K+2)*Y(1,L+2)+ALPHA(I,K+3)*         SPIKEHF    988
           1Y(1,L+3)+ALPHA(I,K+4)*Y(1,L+4)+ALPHA(I,K+5)*Y(1,L+5)+ALPHA(I,K+6)*         SPIKEHF    989
           2Y(1,L+6)+ALPHA(I,K+7)*Y(1,L+7)                                             SPIKEHF    990
  270       DERV1Y(1)=DERV1Y(1)+SIGNL(1)                                               SPIKEHF    991
            DERV1Y(9)=DERV1Y(9)-SIGNL(8)                                               SPIKEHF    992
            DO 24 I=2,8                                                                SPIKEHF    993
         24 DERV1Y(I)=DERV1Y(I)+SIGNL(I)-SIGNL(I-1)                                    SPIKEHF    994
      C                                                                                SPIKEHF    995
  275 C CALCULATE OUTPUT POWER                                                         SPIKEHF    996
      C                                                                                SPIKEHF    997
      C     MC*AVAGADRO NO. = 2.85912 CAL-CM/MOLE                                      SPIKEHF    998
            CONST=2.85912*THGAIN                                                       SPIKEHF    999
            PL=0.                                                                      SPIKEHF   1000
  280       DO 25 I=1,8                                                              SPIKEHF   1001
            K=JMAX(I)-4                                                              SPIKEHF   1002
            L=7*I+16                                                                 SPIKEHF   1003
            DO 25 J=1,7                                                              SPIKEHF   1004
         25 PL=PL+Y(1,L+J)*MC(I,K+J)                                                 SPIKEHF   1005
  285       PL=PL*CONST                                                              SPIKEHF   1006
      C                                                                              SPIKEHF   1007
      C TEMPERATURE DERIVATIVE                                                       SPIKEHF   1008
      C                                                                              SPIKEHF   1009
            AIT=Y(1,23)/100.+.5                                                      SPIKEHF   1010
  290       IT=IFIX(AIT)                                                             SPIKEHF   1011
            CVSUM=2.981*(HE+AR+Y(1,17))+CVN2(IT)*N2+CVSF6(IT)*SF6+5.076*(Y(1,1     SPIKEHF   1012
           118)+Y(1,19)+Y(1,20))+5.020*(Y(1,1)+Y(1,2)+Y(1,3)+Y(1,4)+Y(1,5)+Y(1,    SPIKEHF   1013
           126)+Y(1,7)+Y(1,8)+Y(1,9))+CVF(IT)*Y(1,21)+CVF2(IT)*Y(1,22)              SPIKEHF   1014
            CVSUM=CVSUM+CVC(IT)*Y(1,15)+CVO2(IT)*Y(1,16)+CVOH(IT)*Y(1,80)+CVH2     SPIKEHF   1015 |O2
  295       10(IT)*Y(1,81)+CVHO2(IT)*Y(1,83)                                         SPIKEHF   1016
            ETHLPY=((EHPYH(IT)+52.103)-(EHPYF(IT)+18.900))*DERV1Y(17)+(EHPYF2(      SPIKEHF   1017
           1IT))*DERV1Y(22)+(EHPYH2(IT))*DERV1Y(18)+(EHPYH2(IT)+11.889)*DERV1Y      SPIKEHF   1018
           2(19)+(EHPYH2(IT)+23.112)*DERV1Y(20)+(EHPYHF(IT)-64.800)*DERV1Y(1)+     SPIKEHF   1019
           3(EHPYHF(IT)-53.473)*DERV1Y(2)+(EHPYHF(IT)-42.638)*DERV1Y(3)+(EHPYH     SPIKEHF   1020
  300      4F(IT)-32.282)*DERV1Y(4)+(EHPYHF(IT)-22.392)*DERV1Y(5)+(EHPYHF(IT)-     SPIKEHF   1021
           512.959)*DERV1Y(6)+(EHPYHF(IT)-3.973)*DERV1Y(7)+(EHPYHF(IT)+4.572)*     SPIKEHF   1022
           6DERV1Y(8)+(EHPYHF(IT)+12.660)*DERV1Y(9)                                  SPIKEHF   1023
            ETHLPY=ETHLPY+(EHPYO(IT)+69.959)*DERV1Y(15)+EHPYO2(IT)*DERV1Y(16)+     SPIKEHF   1024 |O2
           1(EHPYOH(IT)+9.31)*DERV1Y(80)+(EHPYH2O(IT)-57.789)*DERV1Y(81)+(EHPY     SPIKEHF   1025
  305      2HO2(IT)+5.)*DERV1Y(83)                                                   SPIKEHF   1026
            ETHLPY=ETHLPY*1.E+3                                                      SPIKEHF   1027
            DERV1Y(23)=-(PL-PPHOTC+ETHLPY)/CVSUM                                     SPIKEHF   1028
            DO 26 I=1,8                                                              SPIKEHF   1029
            L=7*I+16                                                                 SPIKEHF   1030
  310       K=JMAX(I)-4                                                              SPIKEHF   1031
            DO 26 J=1,7                                                              SPIKEHF   1032
         26 DERV1Y(L+J)=(ALPHA(I,K+J)-THGAIN)*2.997925E+10*Y(1,L+J)*LRATIC           SPIKEHF   1033
            DO 27 I=24,79                                                            SPIKEHF   1034
         27 IF (Y(1,I).LE.FLUX.AND.DERV1Y(I).LT.0.) DERV1Y(I)=0.                     SPIKEHF   1035
  315       RETURN                                                                   SPIKEHF   1036
            END                                                                      SPIKEHF   1037
```


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```
      SUBROUTINE DIFSUB (N,T,Y,SAVE,H,HMIN,HMAX,EPS,MF,YMAX,ERROR,KFLAG,  SPIKEHF  1038
     1JSTART,MAXDEG,PW,KEY)                                               SPIKEHF  1039
      DIMENSION Y(8,N), YMAX(N), SAVE(10,N), ERROR(N), PW(N), A(8), PERT  SPIKEHF  1040
     1ST(7,2,3)                                                           SPIKEHF  1041
      DATA PERTST/2.0,4.5,7.333,10.42,13.7,17.15,1.0,2.0,12.0,24.0,37.89  SPIKEHF  1042
     1,53.33,70.08,87.97,3.0,6.0,9.167,12.5,15.98,1.0,1.0,12.0,24.0,37.8  SPIKEHF  1043
     29,53.33,70.08,87.97,1.0,1.0,1.0,0.5,0.1667,0.04133,0.008267,1.0,1.0,SPIKEHF  1044
     31.0,2.0,1.0,.3157,.07407,.0139/                                     SPIKEHF  1045
      DATA A(2)/-1.0/                                                     SPIKEHF  1046
      IRET=1                                                              SPIKEHF  1047
      KFLAG=1                                                             SPIKEHF  1048
      IF (JSTART.LE.0) GO TO 5                                            SPIKEHF  1049
    1 DO 2 I=1,N                                                          SPIKEHF  1050
      DO 2 J=1,K                                                          SPIKEHF  1051
    2 SAVE(J,I)=Y(J,I)                                                    SPIKEHF  1052
      HOLD=HNEW                                                           SPIKEHF  1053
      IF (H.EQ.HOLD) GO TO 4                                              SPIKEHF  1054
    3 RACUM=H/HOLD                                                        SPIKEHF  1055
      IRET1=1                                                             SPIKEHF  1056
      GO TO 76                                                            SPIKEHF  1057
    4 NQOLD=NQ                                                            SPIKEHF  1058
      TOLD=T                                                              SPIKEHF  1059
      RACUM=1.0                                                           SPIKEHF  1060
      IF (JSTART.GT.0) GO TO 25                                           SPIKEHF  1061
      GO TO 8                                                             SPIKEHF  1062
    5 IF (JSTART.EQ.-1) GO TO 7                                           SPIKEHF  1063
      N2=1                                                                SPIKEHF  1064
      N3=N                                                                SPIKEHF  1065
      N1=N*10                                                             SPIKEHF  1066
      N2=N1+1                                                             SPIKEHF  1067
      N4=N**2                                                             SPIKEHF  1068
      N5=N1+N                                                             SPIKEHF  1069
      N6=N5+1                                                             SPIKEHF  1070
      CALL DIFFUN (T,Y,SAVE(N2,1),1)                                      SPIKEHF  1071
      DO 6 I=1,N                                                          SPIKEHF  1072
      N11=N1+I                                                            SPIKEHF  1073
    6 Y(2,I)=SAVE(N11,1)*H                                                SPIKEHF  1074
      HNEW=H                                                              SPIKEHF  1075
      K=2                                                                 SPIKEHF  1076
      GO TO 1                                                             SPIKEHF  1077
    7 IF (NQ.EQ.NQOLD) JSTART=1                                           SPIKEHF  1078
      T=TOLD                                                              SPIKEHF  1079
      NQ=NQOLD                                                            SPIKEHF  1080
      K=NQ+1                                                              SPIKEHF  1081
      GO TO 3                                                             SPIKEHF  1082
    8 IF (MF.EQ.0) GO TO 9                                                SPIKEHF  1083
      IF (NQ.GT.6) GO TO 10                                               SPIKEHF  1084
      GO TO (10,19,20,21,22,23), NQ                                       SPIKEHF  1085
    9 IF (NQ.GT.7) GO TO 10                                               SPIKEHF  1086
      GO TO (11,12,13,14,15,16,17), NQ                                    SPIKEHF  1087
   10 KFLAG=-2                                                            SPIKEHF  1088
      RETURN                                                              SPIKEHF  1089
   11 A(1)=-1.0                                                           SPIKEHF  1090
```


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```
                GO TO 24
     55    12   A(1)=-0.5000000000000000
               A(3)=-0.5000000000000000
                GO TO 24
           13   A(1)=-0.4166666666666667
               A(3)=-0.7500000000000000000000000000
     60        A(4)=-0.1666666666666667
                GO TO 24
           14   A(1)=-0.3750000000000000000000000000
               A(3)=-0.9166666666666667
               A(4)=-0.3333333333333333
     65        A(5)=-0.0416666666666667
                GO TO 24
           15   A(1)=-0.3486111111111111111111111111
               A(3)=-1.0416666666666667
               A(4)=-0.4861111111111111111111111111
     70        A(5)=-0.1041666666666667
               A(6)=-0.0083333333333333333333333333
                GO TO 24
           16   A(1)=-0.3298611111111111111111111111
               A(3)=-1.1416666666666666666666666667
     75        A(4)=-0.6250000000000000
               A(5)=-0.1770833333333333333333333333
               A(6)=-0.0250000000000000000000000000
               A(7)=-0.0013888888888888888888888889
                GO TO 24
     80    17   A(1)=-0.3155913312169312
               A(3)=-1.2350000000000
               A(4)=-0.7518518518518519
               A(5)=-0.2552083333333333333
               A(6)=-0.0486111111111111111111111111
     85        A(7)=-0.0048611111111111111111111111
               A(8)=-0.0019841269841269841269841269
                GO TO 24
           18   A(1)=-1.0000
                GO TO 24
     90    19   A(1)=-0.6666666666666666667
               A(3)=-0.3333333333333333333333333333
                GO TO 24
           20   A(1)=-0.5454545454545454545454545454
               A(3)=A(1)
     95        A(4)=-0.0909090909090909090909090909
                GO TO 24
           21   A(1)=-0.4800000000000000000000000000
               A(3)=-0.7000000000000000
               A(4)=-0.2000000000000000000000000000
    100        A(5)=-0.0200000000000000000000000000
                GO TO 24
           22   A(1)=-0.4379562043795662
               A(3)=-0.8211678832116788
               A(4)=-0.3102189781021898
    105        A(5)=-0.0547445255474526
               A(6)=-0.0036496350364963504
```

```
SPIKEHF  1091
SPIKEHF  1092
SPIKEHF  1093
SPIKEHF  1094
SPIKEHF  1095
SPIKEHF  1096
SPIKEHF  1097
SPIKEHF  1098
SPIKEHF  1099
SPIKEHF  1100
SPIKEHF  1101
SPIKEHF  1102
SPIKEHF  1103
SPIKEHF  1104
SPIKEHF  1105
SPIKEHF  1106
SPIKEHF  1107
SPIKEHF  1108
SPIKEHF  1109
SPIKEHF  1110
SPIKEHF  1111
SPIKEHF  1112
SPIKEHF  1113
SPIKEHF  1114
SPIKEHF  1115
SPIKEHF  1116
SPIKEHF  1117
SPIKEHF  1118
SPIKEHF  1119
SPIKEHF  1120
SPIKEHF  1121
SPIKEHF  1122
SPIKEHF  1123
SPIKEHF  1124
SPIKEHF  1125
SPIKEHF  1126
SPIKEHF  1127
SPIKEHF  1128
SPIKEHF  1129
SPIKEHF  1130
SPIKEHF  1131
SPIKEHF  1132
SPIKEHF  1133
SPIKEHF  1134
SPIKEHF  1135
SPIKEHF  1136
SPIKEHF  1137
SPIKEHF  1138
SPIKEHF  1139
SPIKEHF  1140
SPIKEHF  1141
SPIKEHF  1142
SPIKEHF  1143
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                      GO TO 24                                                  SPIKEHF  1144
                23    A(1)=-0.4081632653061225                                  SPIKEHF  1145
                      A(3)=-0.9206349206349206                                  SPIKEHF  1146
          110         A(4)=-0.4166666666666667                                  SPIKEHF  1147
                      A(5)=-0.0992063492063492                                  SPIKEHF  1148
                      A(6)=-0.0119047619047619                                  SPIKEHF  1149
                      A(7)=-0.0005668934240362812                               SPIKEHF  1150
                24    K=NQ+1                                                    SPIKEHF  1151
          115         IDOUB=K                                                   SPIKEHF  1152
                      MTYP=(4-MF)/2                                             SPIKEHF  1153
                      ENQ2=.5/FLOAT(NQ+1)                                       SPIKEHF  1154
                      ENQ3=.5/FLOAT(NQ+2)                                       SPIKEHF  1155
                      ENQ1=.5/FLOAT(NQ)                                         SPIKEHF  1156
                      PEPSH=EPS                                                 SPIKEHF  1157
          120         EUP=(PERTST(NQ,MTYP,2)*PEPSH)**2                          SPIKEHF  1158
                      E=(PERTST(NQ,MTYP,1)*PEPSH)**2                            SPIKEHF  1159
                      EDWN=(PERTST(NQ,MTYP,3)*PEPSH)**2                         SPIKEHF  1160
                      IF (EDWN.EQ.0) GO TO 79                                   SPIKEHF  1161
          125         BND=EPS*ENQ3/FLOAT(N)                                     SPIKEHF  1162
                      IWEVAL=MF                                                 SPIKEHF  1163
                      GO TO (25,69), IRET                                       SPIKEHF  1164
                25    T=T+H                                                     SPIKEHF  1165
                      DO 26 J=2,K                                               SPIKEHF  1166
          130         DO 26 J1=J,K                                              SPIKEHF  1167
                      J2=K-J1+J-1                                               SPIKEHF  1168
                      DO 26 I=1,N                                               SPIKEHF  1169
                26    Y(J2,I)=Y(J2,I)+Y(J2+1,I)                                 SPIKEHF  1170
                      DO 27 I=1,KEY                                             SPIKEHF  1171
          135         IF (I.LT.80.AND.I.GT.23) GO TO 27                         SPIKEHF  1172
                      IF (Y(1,I).LT.0.) GO TO 46                                SPIKEHF  1173
                27    CONTINUE                                                  SPIKEHF  1174
                      DO 28 I=1,N                                               SPIKEHF  1175
                28    ERROR(I)=0.0                                              SPIKEHF  1176
          140         DO 45 L=1,3                                               SPIKEHF  1177
                      CALL DIFFUN (T,Y,SAVE(N2,1),1)                            SPIKEHF  1178
                      IF (IWEVAL.LT.1) GO TO 36                                 SPIKEHF  1179
                      IF (MF.EQ.2) GO TO 32                                     SPIKEHF  1180
                      CALL PEDERV (T,Y,PW,N3)                                   SPIKEHF  1181
          145         R=A(1)*H                                                  SPIKEHF  1182
                      DO 29 I=1,N4                                              SPIKEHF  1183
                29    PW(I)=PW(I)*R                                             SPIKEHF  1184
                30    N11=N3+1                                                  SPIKEHF  1185
                      N12=N*N11-N3                                              SPIKEHF  1186
          150         DO 31 I=1,N12,N11                                         SPIKEHF  1187
                31    PW(I)=1.0+PW(I)                                           SPIKEHF  1188
                      IWEVAL=-1                                                 SPIKEHF  1189
                      CALL MATINV (PW,N,N3,J1)                                  SPIKEHF  1190
                      IF (J1.GT.0) GO TO 36                                     SPIKEHF  1191
          155         GO TO 46                                                  SPIKEHF  1192
                32    DO 33 I=1,N                                               SPIKEHF  1193
                33    SAVE(9,I)=Y(1,I)                                          SPIKEHF  1194
                      DO 35 J=1,N                                               SPIKEHF  1195
                      R=EPS*AMAX1(EPS,ABS(SAVE(9,J)))                           SPIKEHF  1196
```

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      SUBROUTINE DIFSUB                                                                 12/21/77

  160                 Y(1,J)=Y(1,J)+R                                                   SPIKEHF  1197
                      D=A(1)*H/R                                                        SPIKEHF  1198
                      CALL  DIFFUN (T,Y,SAVE(N6,1),1)                                   SPIKEHF  1199
                      DO 34  I=1,N                                                      SPIKEHF  1200
                      N11=I+(J-1)*N3                                                    SPIKEHF  1201
  165                 N12=N5+I                                                          SPIKEHF  1202
                      N13=N1+I                                                          SPIKEHF  1203
                34    PW(N11)=(SAVE(N12,1)-SAVE(N13,1))*D                               SPIKEHF  1204
                35    Y(1,J)=SAVE(9,J)                                                  SPIKEHF  1205
                      GO TO 30                                                          SPIKEHF  1206
  170           36    IF (MF.NE.0) GO TO 38                                             SPIKEHF  1207
                      DO 37  I=1,N                                                      SPIKEHF  1208
                      N11=N1+I                                                          SPIKEHF  1209
                37    SAVE(9,I)=Y(2,I)-SAVE(N11,1)*H                                    SPIKEHF  1210
                      GO TO 42                                                          SPIKEHF  1211
  175           38    DO 39  I=1,N                                                      SPIKEHF  1212
                      N11=N5+I                                                          SPIKEHF  1213
                      N12=N1+I                                                          SPIKEHF  1214
                39    SAVE(N11,1)=Y(2,I)-SAVE(N12,1)*H                                  SPIKEHF  1215
                      DO 41  I=1,N                                                      SPIKEHF  1216
  180                 D=0.0                                                             SPIKEHF  1217
                      DO 40  J=1,N                                                      SPIKEHF  1218
                      N11=I+(J-1)*N3                                                    SPIKEHF  1219
                      N12=N5+J                                                          SPIKEHF  1220
                40    D=D+PW(N11)*SAVE(N12,1)                                           SPIKEHF  1221
  185           41    SAVE(9,I)=D                                                       SPIKEHF  1222
                42    NT=N                                                              SPIKEHF  1223
                      DO 43  I=1,N                                                      SPIKEHF  1224
                      Y(1,I)=Y(1,I)+A(1)*SAVE(9,I)                                      SPIKEHF  1225
                      Y(2,I)=Y(2,I)-SAVE(9,I)                                           SPIKEHF  1226
  190                 ERROR(I)=ERROR(I)+SAVE(9,I)                                       SPIKEHF  1227
                      IF (ABS(SAVE(9,I)).LE.(BNO*YMAX(I))) NT=NT-1                      SPIKEHF  1228
                43    CONTINUE                                                          SPIKEHF  1229
                      DO 44  I=1,KEY                                                    SPIKEHF  1230
                      IF (I.LT.80.AND.I.GT.23) GO TO 44                                 SPIKEHF  1231
  195                 IF (Y(1,I).LT.0.) GO TO 45                                        SPIKEHF  1232
                44    CONTINUE                                                          SPIKEHF  1233
                      IF (NT.LE.0) GO TO 50                                             SPIKEHF  1234
                45    CONTINUE                                                          SPIKEHF  1235
                46    T=T-H                                                             SPIKEHF  1236
  200                 IF ((H.LE.(HMIN*1.00001)).AND.((IWEVAL-MTYP).LT.-1)) GO TO 47     SPIKEHF  1237
                      IF ((MF.EQ.0).OR.(IWEVAL.NE.1)) RACUM=RACUM*0.2500                SPIKEHF  1238
                      IWEVAL=MF                                                         SPIKEHF  1239
                      IRET1=2                                                           SPIKEHF  1240
                      GO TO 76                                                          SPIKEHF  1241
  205           47    KFLAG=-3                                                          SPIKEHF  1242
                      PRINT 80, H,HMIN,IWEVAL,MTYP,RACUM,HOLD,HMAX                      SPIKEHF  1243
                48    DO 49  I=1,N                                                      SPIKEHF  1244
                      DO 49  J=1,K                                                      SPIKEHF  1245
                49    Y(J,I)=SAVE(J,I)                                                  SPIKEHF  1246
  210                 H=HOLD                                                            SPIKEHF  1247
                      NQ=NQOLD                                                          SPIKEHF  1248
                      JSTART=NQ                                                         SPIKEHF  1249
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                      RETURN                                                    SPIKEHF  1250
                50    D=0.0                                                     SPIKEHF  1251
215                   DO 51 I=1,N                                               SPIKEHF  1252
                51    D=D+(ERROR(I)/YMAX(I))**2                                 SPIKEHF  1253
                      IWEVAL=0                                                  SPIKEHF  1254
                      IF (D.GT.E) GO TO 55                                      SPIKEHF  1255
                      IF (K.LT.3) GO TO 53                                      SPIKEHF  1256
220                   DO 52 J=3,K                                               SPIKEHF  1257
                      DO 52 I=1,N                                               SPIKEHF  1258
                52    Y(J,I)=Y(J,I)+A(J)*ERROR(I)                               SPIKEHF  1259
                53    KFLAG=+1                                                  SPIKEHF  1260
                      HNEW=H                                                    SPIKEHF  1261
225                   IF (IDOUB.LE.1) GO TO 56                                  SPIKEHF  1262
                      IDOUB=IDOUB-1                                             SPIKEHF  1263
                      IF (IDOUB.GT.1) GO TO 71                                  SPIKEHF  1264
                      DO 54 I=1,N                                               SPIKEHF  1265
                54    SAVE(10,I)=ERROR(I)                                       SPIKEHF  1266
230                   GO TO 71                                                  SPIKEHF  1267
                55    KFLAG=KFLAG-2                                             SPIKEHF  1268
                      IF (H.LE.(HMIN*1.00001)) GO TO 75                         SPIKEHF  1269
                      T=TOLD                                                    SPIKEHF  1270
                      IF (KFLAG.LE.-5) GO TO 73                                 SPIKEHF  1271
235             56    PR2=(D/E)**ENQ2*1.2                                       SPIKEHF  1272
                      PR3=1.E+20                                                SPIKEHF  1273
                      IF ((NQ.GE.MAXDER).OR.(KFLAG.LE.-1)) GO TO 58             SPIKEHF  1274
                      D=0.0                                                     SPIKEHF  1275
                      DO 57 I=1,N                                               SPIKEHF  1276
240             57    D=D+((ERROR(I)-SAVE(10,I))/YMAX(I))**2                    SPIKEHF  1277
                      PR3=(D/EUP)**ENQ3*1.4                                     SPIKEHF  1278
                58    PR1=1.E+20                                                SPIKEHF  1279
                      IF (NQ.LE.1) GO TO 60                                     SPIKEHF  1280
                      D=0.0                                                     SPIKEHF  1281
245                   DO 59 I=1,N                                               SPIKEHF  1282
                59    D=D+(Y(K,I)/YMAX(I))**2                                   SPIKEHF  1283
                      PR1=(D/EDWN)**ENQ1*1.3                                    SPIKEHF  1284
                60    CONTINUE                                                  SPIKEHF  1285
                      IF (PR2.LE.PR3) GO TO 66                                  SPIKEHF  1286
250                   IF (PR3.LT.PR1) GO TO 67                                  SPIKEHF  1287
                61    R=1.0/AMAX1(PR1,1.E-4)                                    SPIKEHF  1288
                      NEWQ=NQ-1                                                 SPIKEHF  1289
                62    IDOUB=10                                                  SPIKEHF  1290
                      IF ((KFLAG.EQ.1).AND.(R.LT.(1.1))) GO TO 71               SPIKEHF  1291
255                   IF (NEWQ.LE.NQ) GO TO 64                                  SPIKEHF  1292
                      DO 63 I=1,N                                               SPIKEHF  1293
                63    Y(NEWQ+1,I)=ERROR(I)*A(K)/FLOAT(K)                        SPIKEHF  1294
                64    K=NEWQ+1                                                  SPIKEHF  1295
                      IF (KFLAG.EQ.1) GO TO 68                                  SPIKEHF  1296
260                   RACUM=RACUM*R                                             SPIKEHF  1297
                      IRET1=3                                                   SPIKEHF  1298
                      GO TO 76                                                  SPIKEHF  1299
                65    IF (NEWQ.EQ.NQ) GO TO 25                                  SPIKEHF  1300
                      NQ=NEWQ                                                   SPIKEHF  1301
265                   GO TO 8                                                   SPIKEHF  1302
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```
                66    IF (PR2.GT.PR1) GO TO 61                                  SPIKEHF  1303
                      NEWQ=NQ                                                   SPIKEHF  1304
                      R=1.0/AMAX1(PR2,1.E-4)                                    SPIKEHF  1305
                      GO TO 62                                                  SPIKEHF  1306
278             67    R=1.0/AMAX1(PR3,1.E-4)                                    SPIKEHF  1307
                      NEWQ=NQ+1                                                 SPIKEHF  1308
                      GO TO 62                                                  SPIKEHF  1309
                68    IRET=2                                                    SPIKEHF  1310
                      R=AMIN1(R,HMAX/ABS(H))                                    SPIKEHF  1311
275                   H=H*R                                                     SPIKEHF  1312
                      HNEW=H                                                    SPIKEHF  1313
                      IF (NQ.EQ.NEWQ) GO TO 69                                  SPIKEHF  1314
                      NQ=NEWQ                                                   SPIKEHF  1315
                      GO TO 8                                                   SPIKEHF  1316
280             69    R1=1.0                                                    SPIKEHF  1317
                      DO 70 J=2,K                                               SPIKEHF  1318
                      R1=R1*R                                                   SPIKEHF  1319
                      DO 70 I=1,N                                               SPIKEHF  1320
                70    Y(J,I)=Y(J,I)*R1                                          SPIKEHF  1321
285                   IDOUB=K                                                   SPIKEHF  1322
                71    DO 72 I=1,N                                               SPIKEHF  1323
                72    YMAX(I)=AMAX1(YMAX(I),ABS(Y(1,I)))                        SPIKEHF  1324
                      JSTART=NQ                                                 SPIKEHF  1325
                      RETURN                                                    SPIKEHF  1326
290             73    IF (NQ.EQ.1) GO TO 79                                     SPIKEHF  1327
                      CALL DIFFUN (T,Y,SAVE(N2,1),1)                            SPIKEHF  1328
                      R=H/HOLD                                                  SPIKEHF  1329
                      DO 74 I=1,N                                               SPIKEHF  1330
                      Y(1,I)=SAVE(1,I)                                          SPIKEHF  1331
295                   N11=N1+I                                                  SPIKEHF  1332
                      SAVE(2,I)=HOLD*SAVE(N11,1)                                SPIKEHF  1333
                74    Y(2,I)=SAVE(2,I)*R                                        SPIKEHF  1334
                      NQ=1                                                      SPIKEHF  1335
                      KFLAG=1                                                   SPIKEHF  1336
300                   GO TO 8                                                   SPIKEHF  1337
                75    KFLAG=-1                                                  SPIKEHF  1338
                      HNEW=H                                                    SPIKEHF  1339
                      JSTART=NQ                                                 SPIKEHF  1340
                      RETURN                                                    SPIKEHF  1341
305             76    RACUM=AMAX1(ABS(HMIN/HOLD),RACUM)                         SPIKEHF  1342
                      RACUM=AMIN1(RACUM,ABS(HMAX/HOLD))                         SPIKEHF  1343
                      R1=1.0                                                    SPIKEHF  1344
                      DO 77 J=2,K                                               SPIKEHF  1345
                      R1=R1*RACUM                                               SPIKEHF  1346
310                   DO 77 I=1,N                                               SPIKEHF  1347
                77    Y(J,I)=SAVE(J,I)*R1                                       SPIKEHF  1348
                      H=HOLD*RACUM                                              SPIKEHF  1349
                      DO 78 I=1,N                                               SPIKEHF  1350
                78    Y(1,I)=SAVE(1,I)                                          SPIKEHF  1351
315                   IDOUB=K                                                   SPIKEHF  1352
                      GO TO (4,25,65), IRET                                     SPIKEHF  1353
                79    KFLAG=-4                                                  SPIKEHF  1354
                      PRINT 80, H,HMIN,IWEVAL,MTYP,RACUM,HOLD,T                 SPIKEHF  1355
                      GO TO 48                                                  SPIKEHF  1356
320             C                                                               SPIKEHF  1357
                80    FORMAT (1H1/2E15.5,2I5,3E15.5////)                        SPIKEHF  1358
                      END                                                       SPIKEHF  1359
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SUBROUTINE RATE                                                    12/21/77

 1              SUBROUTINE RATE (TEMP)                                  SPIKEHF  1360
                COMMON /DIFSUB/ YMAX(100),SAVE(12,100),ERROR(100),PW(10000)  SPIKEHF  1361
                COMMON /SPECT/ E(10,31),MC(9,10),B(9,10),Q(9,61)        SPIKEHF  1362
                COMMON /CV/ CVH2(17),CVF(17),CVF2(17),CVHF(17),CVSF6(17),CVN2(17)  SPIKEHF  1363
 5              COMMON /CVOXG/ CVO(17),CVC2(17),CVCH(17),CVH2O(17),CVHO2(17)  SPIKEHF  1364
                COMMON /EMPY/ EMPYH(17),EMPYH2(17),EMPYF(17),EMPYF2(17),EMPYHF(17)  SPIKEHF  1365
                COMMON /EMPYOXG/ EMPYO(17),EMPYO2(17),EMPYOH(17),EMPYH2O(17),EMPYH  SPIKEHF  1366
               1O2(17)                                                  SPIKEHF  1367
                COMMON /NUMVAR/ NVAR,NFVAR,MFLAG,MFLAG,NEQN             SPIKEHF  1368
10              COMMON /GAIN/ ALFHA(8,15),THGAIN                        SPIKEHF  1369
                COMMON /DERV/ BOLTZ(7,13),MFBJ(7,13),FLUX,TAU(7,13),SIGNL(8)  SPIKEHF  1370
                COMMON /RATES/ KFR(186),KBR(186),RCTF(186),RCTB(186),RF(186)  SPIKEHF  1371
                COMMON /DILUENT/ SF6,AF,HE,N2                           SPIKEHF  1372
                COMMON /POWER/ PLINE(8,15),ELINE(8,15),PL               SPIKEHF  1373
15              COMMON /MISC/ LRATIO,JMAX(8)                            SPIKEHF  1374
                REAL KFR,KBR,N2,LRATIO                                  SPIKEHF  1375
                J=0                                                     SPIKEHF  1376
                DO 1 I=143,150                                          SPIKEHF  1377
                J=J+1                                                   SPIKEHF  1378
20              KFR(I)=(FLOAT(J)**2.5)*(11.*TEMP**3+2.4E9)              SPIKEHF  1379
          1     KBR(I)=0.                                               SPIKEHF  1380
                RETURN                                                  SPIKEHF  1381
                END                                                     SPIKEHF  1382


SUBROUTINE MATINV                                                  12/21/77

 1              SUBROUTINE MATINV (PW,N,M,J)                            SPIKEHF  1383
                RETURN                                                  SPIKEHF  1384
                END                                                     SPIKEHF  1385


SUBROUTINE PEDERV                                                  12/21/77

 1              SUBROUTINE PEDERV (T,Y,PW,M)                            SPIKEHF  1386
                RETURN                                                  SPIKEHF  1387
                END                                                     SPIKEHF  1388
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