A COMPUTER PROGRAM FOR A LINE-BY-LINE CALCULATION OF SPECTRA FROM DIATOMIC MOLECULES AND ATOMS ASSUMING A VOIGT LINE PROFILE

by Ellis E. Whiting, James O. Arnold, and Gilbert C. Lyle

Ames Research Center
Moffett Field, Calif.
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SUMMARY

A Fortran IV computer program for predicting the spectra resulting from
electronic transitions of diatomic molecules and atoms in local thermodynamic
equilibrium is described in detail. Included are instructions for preparing
the input data, a program listing, and complete flow charts. The program pro-
duces a spectrum by accounting for the contribution of each rotational and
atomic line considered. The integrated intensity of each line is distributed
in the spectrum by an approximate Voigt profile. The program can produce
spectra for optically thin gases or for cases where simultaneous emission and
absorption occurs. In addition, the program can compute the spectrum result-
ing from the absorption of incident radiation by a column of cold gas or the
high-temperature, self-absorbed emission spectrum from a nonisothermal gas.
The computed spectrum can be output directly or combined with a slit function
and sensitivity calibration to predict the output of a grating spectrograph or
a fixed wavelength radiometer.

INTRODUCTION

There are many applications in the field of quantitative spectroscopy
where the ability to compute an emission or absorption spectrum is required.
For example, electronic transition moments (or f-numbers) are often determined
by comparing measured and computed intensities (see refs. 1-5). In such an
application, test conditions giving an optically thin gas are usually required
to simplify the problem, although Drake, Tyte, and Nicholls (ref. 5) recently
reported a technique for determining these quantities from strongly self-
absorbed spectra. Detailed spectral computations are also used in predicting
radiative heat transfer in hot-gas environments, in stellar atmosphere cal-
culations, for determining planetary surface pressure from measured line
broadening, and for establishing basic spectroscopic constants.

The task of computing a reasonably accurate spectrum for a mixture of
atoms and diatomic molecules is complicated by the enormously large number
(often tens of thousands) of rotational lines forming the spectrum. In addition,
several kinds of electronic transitions may be involved, each with its
own required set of line strength and wavelength equations. These considera-
tions make it impractical to produce the band spectra from even a simple
diatomic transition, such as \( \text{BeO}(^1\Sigma \rightarrow ^1\Sigma) \), without the aid of an electronic computer. In response to this need, several computer programs have been written to produce synthetic spectra (see, e.g., refs. 5 and 6). However, most programs have been written for specific applications and cannot be applied to more general requirements. The present work was undertaken to develop a computer program applicable, to some degree of approximation, to any "allowed" electronic transition of diatomic molecules and atoms. Specifically, the program has the capability to include the following features in any computation:

1. Parallel transitions \( (\Delta \Lambda = \Lambda' - \Lambda'' = 0) \), in which spin splitting and lambda doubling are ignored (ignoring spin splitting and/or lambda doubling means herein that the total multiplet strength is assumed to reside in a single "effective" line),

2. Perpendicular transitions \( (\Delta \Lambda = \pm 1) \), in which spin splitting and lambda doubling are ignored,

3. \( ^2\Sigma \leftrightarrow ^2\Pi \) transitions, in which lambda doubling is ignored,

4. Atomic lines,

5. Option to terminate rotational-line calculations when the molecule dissociates due to rotation,

6. Option to include the alternation of line intensities for homonuclear molecules,

7. Use of an approximate Voigt profile for the line shape, and

8. Radiative energy transport in a nonisothermal gas.

The restrictions on spin splitting and lambda doubling can be removed with a modest reprogramming effort, but this would result in longer computer run times.

The output options available in the program are:

1. Tabulation of the spontaneous-emission spectrum (i.e., optically thin spectrum) for a 1.0 cm path length,

2. Tabulation of the "true" spectrum, which incorporates spontaneous emission, induced emission, absorption, and externally incident radiation through the equation of radiative transfer,

3. Tabulation of the curve of growth for an arbitrary number of wavelength intervals,

4. Tabulation of the integrated intensity over an arbitrary number of wavelength intervals, and
5. Tabulation of the output signal produced by a radiometer or spectrometer by specifying an instrument calibration. The instrument slit function can be approximated by up to 99 straight-line segments or by a Gaussian curve. The computation can be made at a fixed wavelength to simulate a radiometer or by scanning across any specified wavelength interval to simulate a grating instrument. In the latter case, the sensitivity can be varied as a function of wavelength to accurately simulate a grating-instrument calibration.

The computer program presented is also discussed in reference 7. That reference describes the theoretical and numerical assumptions made in the program, compares computer results with those given by other programs, and demonstrates the flexibility of the program in solving a wide variety of problems. However, that paper does not discuss programming details and, consequently, is not in a useful form for understanding and using the program. This paper provides: (1) a discussion of program operations, (2) a listing of the program statements, (3) detailed flow charts of the program logic, and (4) a guide for preparing the input data necessary to operate the program. It is assumed that the reader has a copy of reference 7 available; therefore, the information contained in that paper will not be reproduced herein.

The program is available from COSMIC, Barrow Hall, University of Georgia, Athens, Georgia. The program package includes the program source decks, an 800 BPI magnetic tape with spectroscopic data for 18 diatomic systems, and the input and output for an extensive program checkout. When requesting this program, refer to Flash Sheet number ARC-10221.

SYMBOLS

<table>
<thead>
<tr>
<th>Commonly Used Notation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALPHA</td>
<td>$\alpha_e$ rotational constant for equilibrium position, cm$^{-1}$</td>
</tr>
<tr>
<td>ALTNAT</td>
<td>alteration factor for homonuclear molecules, dimensionless</td>
</tr>
<tr>
<td>ALTNAT = 0, lines do not alternate in intensity</td>
<td></td>
</tr>
<tr>
<td>ALTNAT = 1, lines with K&quot; odd are strongest</td>
<td></td>
</tr>
<tr>
<td>ALTNAT = 2, lines with K&quot; even are strongest</td>
<td></td>
</tr>
<tr>
<td>ATOMCC</td>
<td>number density of atoms, atoms-cm$^{-3}$</td>
</tr>
<tr>
<td>BE</td>
<td>$B_e$ rotational constant for equilibrium position, cm$^{-1}$</td>
</tr>
<tr>
<td>BE$^{0}$-X</td>
<td>BeO, $B^{1}\Sigma \rightarrow X^{1}\Sigma$ band system for BeO molecule near 4700 Å</td>
</tr>
<tr>
<td>BETAF</td>
<td>$\beta_e$ rotational constant for equilibrium position, cm$^{-1}$</td>
</tr>
<tr>
<td>BLAM</td>
<td>$B^\lambda, B^0_\lambda$ Planck or black-body function, W-cm$^{-2}$-µ$^{-1}$-sr$^{-1}$</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>BV</td>
<td>( B_v ) rotational constant for the vibrational level ( v ), cm(^{-1})</td>
</tr>
<tr>
<td>CAPA</td>
<td>( A ) spin coupling constant, cm(^{-1})</td>
</tr>
<tr>
<td>CAPL</td>
<td>( \Lambda ) quantum number specifying the component of the resultant electronic angular momentum along the internuclear axis, dimensionless</td>
</tr>
<tr>
<td>CH3900</td>
<td>CH, ( ^{2}\Sigma_X - ^{2}\Pi ) band system of CH molecule near 3900 Å</td>
</tr>
<tr>
<td>CH4300</td>
<td>CH, ( ^{2}\Delta_X - ^{2}\Pi ) band system of CH molecule near 4300 Å</td>
</tr>
<tr>
<td>CINT3</td>
<td>INT3 intensity factor defined in equation (12) page 12</td>
</tr>
<tr>
<td>CN V</td>
<td>CN, ( ^{2}\Sigma_X - ^{2}\Sigma ) violet band system of CN molecule</td>
</tr>
<tr>
<td>CN RED</td>
<td>CN, ( ^{2}\Pi_X - ^{2}\Sigma ) red band system of CN molecule</td>
</tr>
<tr>
<td>C(_2)ASDI</td>
<td>C, ( ^{4}\Sigma_X - ^{2}\Pi ) Asundi band system of CO molecule</td>
</tr>
<tr>
<td>C(_2) CT</td>
<td>C, ( ^{4}\Pi - ^{2}\Sigma ) comet tail band system of CO molecule</td>
</tr>
<tr>
<td>C(_2) 4+</td>
<td>C, ( ^{2}\Pi_X - ^{2}\Sigma ) fourth positive band system of CO molecule</td>
</tr>
<tr>
<td>CONST1</td>
<td>{ } constants used in line strength expressions in subroutine S2 PT2 and specified in table I</td>
</tr>
<tr>
<td>CONST2</td>
<td>{ } constants used in Voigt profile expressions and defined in equations on page 11</td>
</tr>
<tr>
<td>CONST3</td>
<td>{ } constant used in line strength expression in subroutine ZERO and defined in equation on page 14</td>
</tr>
<tr>
<td>CSPRD1</td>
<td>{ }</td>
</tr>
<tr>
<td>CSPRD2</td>
<td>{ }</td>
</tr>
<tr>
<td>CSPRD3</td>
<td>{ }</td>
</tr>
<tr>
<td>CSTR</td>
<td>{ }</td>
</tr>
<tr>
<td>C2PHIL</td>
<td>C, ( ^{2}\Pi_{a} \rightarrow ^{2}\Sigma_{a} ) Phillips band system of C(_2) molecule</td>
</tr>
<tr>
<td>C2SWAN</td>
<td>C, ( ^{2}\Sigma_{a} - ^{2}\Pi ) Swan band system of C(_2) molecule</td>
</tr>
<tr>
<td>DE</td>
<td>( D_e ) rotational constant for equilibrium position, cm(^{-1})</td>
</tr>
<tr>
<td>DGEN</td>
<td>( d ) electronic multiplicity, dimensionless</td>
</tr>
<tr>
<td>DELLAM</td>
<td>( \Delta \lambda ) distance between wavelength locations at which spectrum is computed, Å</td>
</tr>
<tr>
<td>DEPTH</td>
<td>( \ell, x ) depth of radiating gas, cm</td>
</tr>
<tr>
<td>DV</td>
<td>( D_v ) rotational constant for the vibrational level ( v ), cm(^{-1})</td>
</tr>
<tr>
<td>DZERO</td>
<td>( D_0 ) dissociation energy referred to the ( v = 0 ) vibrational level, cm(^{-1})</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>-------------</td>
</tr>
<tr>
<td>E, I</td>
<td>line integrated spontaneous emission, W-cm(^{-3})-sr(^{-1})</td>
</tr>
<tr>
<td>G((v))+F(K)</td>
<td>sum of vibrational and rotational energy used in iteration to find KMAX and defined by equation (15) on page 13</td>
</tr>
<tr>
<td>A(_{ul})</td>
<td>Einstein A coefficient, probability of transition, sec(^{-1})-part(^{-1})</td>
</tr>
<tr>
<td>E(<em>{\lambda}, I</em>{\lambda})</td>
<td>spectral intensity distribution of spontaneous emission, W-cm(^{-2})-(\mu)-sr(^{-1})</td>
</tr>
<tr>
<td>q(_{v', v''})</td>
<td>Franck-Condon factor, dimensionless</td>
</tr>
<tr>
<td>IFACTR</td>
<td>integer name of the intensity factor, CINT3, set up in Hollerith mode so that if CINT3 = 0.0 blanks are printed rather than zeros</td>
</tr>
<tr>
<td>E(<em>{\lambda}, B</em>{\lambda})</td>
<td>specific intensity, W-cm(^{-2})-(\mu)-sr(^{-1})</td>
</tr>
<tr>
<td>J</td>
<td>rotational quantum number, dimensionless</td>
</tr>
<tr>
<td>K, N</td>
<td>rotational quantum number without spin, dimensionless</td>
</tr>
<tr>
<td>K(<em>{\min}), K(</em>{\max})</td>
<td>minimum rotational quantum number, dimensionless, maximum rotational quantum number, dimensionless</td>
</tr>
<tr>
<td>(\lambda)</td>
<td>wavelengths specifying incident spectrum array or linear segment slit function, Å</td>
</tr>
<tr>
<td>(\lambda_g)</td>
<td>wavelength locations at which spectrum is computed, Å</td>
</tr>
<tr>
<td>(\lambda_{\min}), (\lambda_{\max})</td>
<td>center of rotational or atomic line or location of center of slit function, Å</td>
</tr>
<tr>
<td>(\lambda_{\min}), (\lambda_{\max})</td>
<td>minimum wavelength in computed spectrum, Å, maximum wavelength in computed spectrum, Å</td>
</tr>
<tr>
<td>(\lambda_{\mathrm{br}})</td>
<td>wavelengths specifying instrument calibration, Å</td>
</tr>
<tr>
<td>(\lambda_{\mathrm{bs}})</td>
<td>wavelengths at which instrument output signal is generated, Å</td>
</tr>
<tr>
<td>(\lambda_{\mathrm{sl}})</td>
<td>starting wavelength for scanning slit or wavelength for fixed linear slit, Å</td>
</tr>
<tr>
<td>(\lambda_{\mathrm{st}})</td>
<td>stopping wavelength for scanning slit, Å</td>
</tr>
<tr>
<td>(\lambda_{\mathrm{s1}})</td>
<td>starting wavelength for spectral integration, Å</td>
</tr>
<tr>
<td>(\lambda_{\mathrm{s2}})</td>
<td>stopping wavelength for spectral integration, Å</td>
</tr>
</tbody>
</table>
LEVELS
number of electronic energy levels for a diatomic molecule

MU $\mu_A$
reduced mass in atomic-weight units

NAME
six-letter (or less) name specifying an atomic or diatomic system

ARRAY
number of points at which spectrum is computed

CENTR
array index in ELAM(M) nearest to center of line being added to spectrum

END
array index in ELAM(M) at which the last contribution of a line is added

INTRV
number of intervals in a case over which the spectrum will be integrated

POINT
number of array elements specifying the slit function. NPOINT = 0 if the slit function is specified by a Gaussian curve

RLAM
number of points specifying the instrument calibration

SLIT
number of slits for which the instrument output signal will be computed

SPRED
one-half the number of places in the spectrum to which a line will be added

START
array index in ELAM(M) at which the first contribution of a line is added

UBAR $\tilde{\nu}$
wave number of a line center, cm$^{-1}$

UBARO $\tilde{\nu}_o(v'v'')$
wave number of a band origin, cm$^{-1}$

USPIN $N,I$
nuclear spin of an atom in a homonuclear diatomic molecule, dimensionless

LBN
Lyman-Birge-Hopfield band system of $N_2$ molecule

1+ $N_2,B^3\Pi\rightarrow A^3\Sigma$
first positive band system of $N_2$ molecule

2+ $N_2,C^3\Pi\rightarrow B^3\Pi$
second positive band system of $N_2$ molecule

1- $N_2,E^2\Sigma\rightarrow X^2\Sigma$
first negative band system of $N_2^+$ molecular ion

B $NO,B^3\Pi\rightarrow X^3\Pi$
beta band system of NO molecule

G $NO,A^2\Sigma\rightarrow X^2\Pi$
gamma band system of NO molecule

SR $O_2,E^3\Sigma\rightarrow X^3\Sigma$
Schuman-Runge band system of $O_2$ molecule

H$3060$ $OH,A^2\Sigma\rightarrow X^2\Pi$
band system of OH molecule near 3060 Å
PARTCC N
number density of molecules, molecules-cm\(^{-3}\)

Q Q
partition function, dimensionless

R r
internuclear distance, cm

RANGE
number of line widths from the line center that a line is added to the spontaneous emission spectrum, integer

RE \(r_e\)
internuclear distance at equilibrium position, cm

RLAM(M)
spectral calibration of scanning slit that multiplies slit function to yield instrument sensitivity

RLAMCL
value of spectral calibration RLAM(M) at slit centerline, LAMCL

RMAX
maximum value of RSLIT(M)

RSLIT(M)
slit function values for linear segment slit function

SCAN
.flag to indicate whether a fixed slit (SCAN \(\neq 1\)) or a scanning slit (SCAN = 1) is specified

SIGN
constant used in line strength expressions in subroutine ONE and in equations (19), (20), and (21) on page 15, dimensionless

SIGNAL
instrument output signal computed in subroutine SLIT, arbitrary units

SIGNAL1 SIGNAL2 SIGNAL3
constants used in line strength expression in subroutine S2 PI2 and in equations (23) and (24) on pages 15 and 16, dimensionless

SIGNAL1 SIGNAL2
constants used in NUBAR expression in subroutine S2 PI2 and in equation (22) on page 15, dimensionless

STEP
wavelength interval between points where the instrument output signal is computed for a scanning slit, Å

SUMRE2 \[\sum |R_e(\bar{F}_{v',v'})/e_o|^2\]
sum of the squares of the dimensionless electronic transition moments. The sum is over all electronic transitions from the upper and lower multiplet levels

TELECT \(T_{\text{elect}}\)
electronic temperature, °K
<table>
<thead>
<tr>
<th>SYMBOL</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>TERM(M)</td>
<td>Te</td>
</tr>
<tr>
<td>TOTALI</td>
<td>T_total</td>
</tr>
<tr>
<td>TROT</td>
<td>T_rot</td>
</tr>
<tr>
<td>TVIB</td>
<td>T_vib</td>
</tr>
<tr>
<td>U</td>
<td>U</td>
</tr>
<tr>
<td>V</td>
<td>v</td>
</tr>
<tr>
<td>WIDTH</td>
<td></td>
</tr>
<tr>
<td>WIDTHG</td>
<td>w_g</td>
</tr>
<tr>
<td>WIDTHL</td>
<td>w_l</td>
</tr>
<tr>
<td>WIDTHV</td>
<td>w_v</td>
</tr>
<tr>
<td>WE</td>
<td>(\omega_e)</td>
</tr>
<tr>
<td>WEKE</td>
<td>(\omega_e^2)</td>
</tr>
<tr>
<td>WEYE</td>
<td>(\omega_e\gamma_e)</td>
</tr>
<tr>
<td>WEZE</td>
<td>(\omega_e^2\gamma_e)</td>
</tr>
<tr>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>U</td>
<td>()',(),(u)</td>
</tr>
<tr>
<td>L</td>
<td>()&quot;,(),(l)</td>
</tr>
<tr>
<td>(\phi)</td>
<td>0</td>
</tr>
</tbody>
</table>

The end result of this program is to produce the "true" spectrum as given by the equation of radiative transfer. Within the computer the "true"
spectrum is generated in two distinct steps. In the first step the spectrum due to spontaneous emission only is computed. This is accomplished by summing the spectral contributions from all included lines at many points within the spectral range considered. For atomic lines this is accomplished entirely within the ATOMIC subroutine. For diatomic molecules the procedure is somewhat more complicated. When a new band system is specified, program control is transferred to the SETUP subroutine. In this subroutine, the spectroscopic constants are read either from cards or from magnetic tape and the partition function, \( Q \), is computed. After these tasks are completed, control is transferred back to the main program where a vibrational band card is read. This card causes control to be transferred to the VU VL subroutine where: (1) the appropriate vibrational constants are computed from the spectroscopic constants, (2) an intensity factor (CINT3) is computed if needed, and (3) the maximum rotational quantum number is found. After these tasks are completed, control is transferred back to the main program, followed by an immediate transfer to the appropriate rotational-structure subroutine, ZERO, ONE, or S2 PI2. Subroutine ZERO applies to parallel transitions, subroutine ONE applies to perpendicular transitions, and subroutine S2 PI2 applies to \( \Sigma \rightarrow \Pi \) or \( \Pi \rightarrow \Sigma \) transitions. In these subroutines, the wavelength and integrated intensity due to spontaneous emission of each rotational line are calculated, the intensity is distributed spectrally into a Voigt profile, and the line is added into the spectrum.

If several vibrational bands are specified for several band systems, the summation process can include tens of thousands of rotational lines. The resultant spectral sum of this multitude of lines, including any atomic lines specified, yields the spontaneous-emission spectrum. If an optically thin spectrum is desired as a final result, it is given directly by the spontaneous-emission spectrum.

The second step in the development of the "true" spectrum is to compute the wavelength-dependent absorption coefficient, including induced emission. As described in reference 7, this function is given directly by dividing the spectral intensities due to spontaneous emission, developed above, by the Planck (or black body) function at the appropriate temperature and wavelengths. The absorption coefficient is then combined with the geometric gas depth and the incident radiation, if specified, in the equation of radiative transfer to give the "true" spectrum.

The generality of the program is greatly enhanced by permitting the "true" spectrum radiating from a gas layer to be used as the incident radiation for a new gas layer. This allows the calculation of the "true" spectrum from a multilayer source, where each layer is specified by a different thermochemical and thermodynamic environment.

Most of the numerical steps performed in the program can be easily understood once the intent of the operation is known. The comment statements in the listing and the description of the theory given in reference 7 should make the intent of most operations clearly evident. There are, however, a few operations that need additional discussion. These are presented in the following sections.
Spontaneous-Emission Spectrum

The procedure for building the spectrum involves several steps. These steps will be easier to understand if the notation illustrated in figure 2 is followed closely during the discussion. A large array (ELAM(M)) with 9000 entries is reserved in the computer core for summing the spectral intensity at many points within the spectral range considered. The minimum (IAMMIN) and maximum (LAMMAX) wavelengths are specified as is the wavelength interval (DELLAM) between points where the spectrum is to be summed. For good spectral resolution, DELLAM is normally selected to be about 1/10 of the narrowest line width at half-height (WIDTHHV) considered in the calculation.

The total number of points at which the spectrum is summed (NARRAY) is limited to 9000. NARRAY is found from IAMMIN, LAMMAX, and DELLAM, and, if NARRAY is greater than 9000, DELLAM is changed so that NARRAY is equal to 9000. LAMMAX is always recomputed to ensure that it is exactly an even increment of DELLAM from IAMMIN. For this reason, the value of LAMMAX used and output by the program may be slightly less than the value input.

The contributions from each rotational and atomic line to the spontaneous emission spectrum are added into the ELAM(M) array by the following procedure. The array index number nearest to the line center (NCENTR) is found from (refer to fig. 2)

$$
NCENTR = \left(\frac{LAMCL - IAMMIN}{DELLAM} + 1.5\right)_{\text{truncated}}
$$

where LAMCL is the wavelength of the line center, and the characteristic of Fortran IV to convert real numbers into integer numbers by rounding down (truncating) has been used.

Theoretically, each line makes a contribution to the spectrum at all wavelengths. Beyond some distance from the line center, however, the contribution of the line to the spectral intensity is very small. Therefore, computer run time can be reduced considerably, with slight loss in accuracy, by adding each line into the spectrum for only a limited distance from the line center. In the program, this distance is specified by RANGE, in terms of a given number of line widths.

If RANGE is input as zero (or the card field is left blank) then RANGE is set as follows: For a pure Gaussian line profile, the spontaneous-emission intensity is less than $10^{-11}$ of the peak line intensity only three line widths from the line center. Therefore, RANGE = 3.0 is considered adequate for this case. For a Lorentzian or Voigt line profile the intensity in the wings is much stronger than for a Gaussian profile, and RANGE is increased to 5.0 for these cases. This limitation results in approximately 5 percent of the spontaneous integrated intensity being excluded from the computation for a pure Lorentzian line profile.

The number of entries in the ELAM(M) array from the location defined by NCENTR, to which contributions from a given line are added, is
The array indices that define the first \((N_{\text{START}})\) and the last \((N_{\text{END}})\) entries in the \(ELAM(M)\) array to which a contribution from a line is added is

\[
N_{\text{START}} = NCENTR - NSPRED
\]

\[
N_{\text{END}} = NCENTR + NSPRED
\]

These indices provide limits for a simple \(DO\) loop, involving the line-profile expression (see refs. 7 and 8), which adds the contributions from each line to the correct locations in the \(ELAM(M)\) array, and hence forms the spontaneous-emission spectrum. In partial Fortran IV notation, the line-profile expression from reference 8 can be written

\[
\begin{align*}
ELAM(M) &= E \left[ CSPRD1 \cdot e^{-2.772 \cdot CSPRD3^2} + \frac{CSPRD2}{1 + 4 \cdot CSPRD3^2} \right. \\
&\left. + 0.016 \cdot CSPRD2 \left(1 - \frac{\text{WIDTHL}}{\text{WIDTHHV}}\right) e^{-0.4 \cdot CSPRD3^2} \cdot \frac{10.0}{10 + CSPRD3^2} \right]
\end{align*}
\]

where \(E\) is the integrated spontaneous emission of the line and

\[
CSPRD1 = \frac{\left[1 - (\text{WIDTHL}/\text{WIDTHHV})\right] \cdot 10^4}{\text{WIDTHHV}[1.065 + 0.447(\text{WIDTHL}/\text{WIDTHHV}) + 0.058(\text{WIDTHL}/\text{WIDTHHV})^2]}
\]

\[
CSPRD2 = \frac{(\text{WIDTHL}/\text{WIDTHHV}) \cdot 10^4}{\text{WIDTHHV}[1.065 + 0.447(\text{WIDTHL}/\text{WIDTHHV}) + 0.058(\text{WIDTHL}/\text{WIDTHHV})^2]}
\]

\[
CSPRD3 = \left| \frac{\text{LAMBDAL} - \text{LAMCL}}{\text{WIDTHV}} \right|
\]

\(\text{LAMBDAL}\) is the wavelength at which the spectrum is computed

\[
= \text{LAMMIN} + (M - 1) \cdot \text{DELLAM}
\]

**Intensity Factor**

The first major step taken in the program for any spectral computation is to generate the spontaneous-emission spectrum as outlined above. When spontaneous emission from a cold gas is computed, however, the intensities are
numerically small because of the low concentration of molecules in the upper state. The expression for the number of molecules in the upper state is given by (see ref. 7)

\[
N_u = \frac{N_d (2J' + 1)e^{-\frac{\hbar c}{k} \left( \frac{T_e}{T_{\text{elect}}} + \frac{G'}{T_{\text{vib}}} + \frac{F'}{T_{\text{rot}}} \right)}}{Q}
\tag{10}
\]

The exponent will be a large negative number for high term energies and/or low temperatures. For example, in the case of the A^3Π state of CO at room temperature, the electronic and vibrational part of the exponent is approximately -300. The computer cannot recognize numbers less than \(10^{-38} = e^{-37.5}\) and simply equates all numbers less than this value to 0.0. Therefore, a straightforward application of the above equation to CO(4+) at room temperature would produce meaningless numbers.

To overcome this computer-caused limitation, an intensity factor is introduced as follows:

\[
\overline{N}_u = N_u \cdot 10^\text{CINT3} = \frac{N_d (2J' + 1)e^{-\frac{\hbar c}{k} \left( \frac{T_e}{T_{\text{elect}}} + \frac{G'}{T_{\text{vib}}} + \frac{F'}{T_{\text{rot}}} \right)}}{Q} \cdot 2.30259 \cdot \text{CINT3}
\tag{11}
\]

where

\[
\text{CINT3} = \left| \frac{\hbar c}{k} \left( \frac{T_e}{T_{\text{elect}}} + \frac{G'}{T_{\text{vib}}} \right) \right| \text{ truncated}
\tag{12}
\]

From these expressions, it is clear that CINT3 is an even power of 10 that adjusts the numerical value of \(N_u\) into a numerically acceptable regime. Results that include the intensity factor are obviously in error by this factor and it must be removed before the results can be used. When numbers reflecting only spontaneous emission are printed, the correction is applied at the time of printing. For example, suppose an exact intensity of \(3.5 \times 10^{-17}\) should have been computed, but an intensity factor of \(10^{170}\) was applied. The value found by the program is, therefore, \(3.5 \times 10^{-8}\), but is printed as \(3.5 \times 10^{-8} \times 10^{170}\). In printer notation this appears as \(3.5005-08-170\). The intensity factor is printed by using the Hollerith array, IFACTR, so that, when the intensity factor is zero, blanks will appear on the printed output rather than zeros. When the "true" spectrum is computed, the intensity factor is removed from the calculation at the time the absorption coefficient is computed and no further correction is necessary.
Maximum Rotational Quantum Number (KMAX)

A rotating molecule develops a centrifugal force that distorts the potential well. If the nonrotating potential well is described by a Morse potential, then the rotation-dependent potential is given by (see ref. 9)

\[ U = D_e \left[ 1 - e^{-\beta (R - R_e)} \right]^2 + \frac{\hbar K(K + 1)}{8\pi^2 \mu R^2} \tag{13} \]

where

\[ \beta = \left( \frac{2\pi^2 \mu D_e \hbar}{\beta e} \right)^{1/2} \tag{14} \]

\[ \mu = \text{reduced mass, } g \]

The effect of rotation on the potential well can be seen by the curves in figure 3 for HgH taken from reference 9. The molecule will dissociate when the vibrational plus rotational energy equals or exceeds the rotation-induced local maximum in the potential well. The sum of the vibrational and rotational energies is given by

\[ E = \omega_e (v + 1/2) - \omega_x \chi_e (v + 1/2)^2 + \omega_y \psi_e (v + 1/2)^3 + \omega_z \zeta_e (v + 1/2)^4 \]

\[ + B_v K(K + 1) - D_v K^2 (K + 1)^2 \tag{15} \]

Therefore, once a vibrational level has been specified, an iteration scheme is required to find KMAX from equations (13) and (15).

The energy of the local maximum can be found from equation (13) if the rotational quantum number and the internuclear distance (R) at that point are known. The internuclear distance at the local maximum is found for a specified value of K by differentiating equation (13) and equating it to zero, that is,

\[ \frac{dU}{dR} = 2D_e \beta \left[ 1 - e^{-\beta (R - R_e)} \right] e^{-\beta (R - R_e)} - \frac{2\hbar K(K + 1)}{8\pi^2 \mu R^3} = 0 \tag{16} \]

For numerical solution, this equation is rewritten as

\[ f(R) = R^3 \left[ 1 - e^{-\beta (R - R_e)} \right] e^{-\beta (R - R_e)} - \frac{\hbar K(K + 1)}{8\pi^2 \mu D_e \beta} = g(K) \tag{17} \]

and is illustrated in figure 4.

\[ ^1 \text{In fact, some predissociation will occur at lower energies due to a wave mechanical passage through the potential barrier, but this effect is ignored in the present program.} \]
The value of $R$ at the local maximum, $R'$, is found by stepping $R$ from its equilibrium value ($R_e$) by fixed increments ($0.1 \times 10^{-6} \text{ cm}$) until $f(R)$ exceeds and then falls below $g(K)$; $R'$ is then found by interpolating to $f(R) = g(K)$. If $f(R)$ passes its maximum before $g(K)$ is reached, the rotational quantum number is too large and rotational dissociation would have occurred. A local maximum in the potential well does not exist in this case (see curve for $K = 40$ in fig. 3), but a value of $R$ at or near the peak of the $f(R)$ curve is chosen for the iteration.

Once the internuclear distance for the local maximum is found (at the specified rotational quantum number) it is combined with the vibrational quantum number to compute the values of $U$ and $E$ from equations (13) and (15). When the iteration has converged, $U$ will be nearly equal to $E$, and hence the difference $U - E$ is a good criterion to guide the iteration process. A representative plot of $U - E$ as a function of $K$ is shown in figure 5. The desired iteration point is obviously the first root of this function.

The first iteration is begun with $K = 50$, and the associated value of $R'$ is found as outlined above; $K$ is then increased in increments of 20, holding $R$ fixed until $U \leq E$. Then, by interpolating to $U - E = 0$, a new value of $K$ is found for the second iteration. A new value of $R'$ is found from the new $K$ value, which, in turn, leads to new values of $U$ and $E$. The new values of $U$, $E$, and $K$, and the prior values of $U$, $E$, and $K$, are used to extrapolate to $U - E = 0$, which determines the next value of $K$. This process is continued until the value of $K$ does not change during an iteration. $K_{\text{MAX}}$ is then set equal to this value of $K$.

The iteration process is very fast, requiring only three or four iterations to converge to the maximum allowed value of $K$. $K_{\text{MAX}}$ values computed in this manner for $O_2$ are in good agreement with the results of reference 10.

The maximum allowed rotational quantum number is found for both the upper and the lower vibrational levels. The value of $K_{\text{MAX}}$ used in the program is the minimum of the upper state value, the lower state value, and the input value if one is specified. If the dissociation energy of an electronic level is not known, $K_{\text{MAX}}$ cannot be found for that level. If $K_{\text{MAX}}$ cannot be found for either level and a value is not input, the program arbitrarily sets $K_{\text{MAX}} = 150$; experience has found this to be a reasonable value except for the halides.

Constants Used in Rotational-Structure Subroutines

(a) Subroutine ZERO

The line-strength expression used for these transitions (i.e., $\Sigma \rightarrow \Sigma$, $\Pi \rightarrow \Pi$, etc.) is (see ref. 7)

$$S = KU + \text{CSTR}$$

where

\[
\begin{align*}
\text{CSTR} &= 0 \quad \text{for the R branch} \\
\text{CSTR} &= 1 \quad \text{for the P branch}
\end{align*}
\]
(b) Subroutine ONE

The line-strength expressions used for these transitions (i.e., Σ → Π, Π → Σ, Π → Δ, etc.) are (see ref. 7)

\[
S(P) = \frac{(KU + 1 - \text{SIGN} \cdot \text{CAPLU})(KU + 2 - \text{SIGN} \cdot \text{CAPLU})}{2(KU + 1)}
\]

(19)

\[
S(Q) = \frac{(KU + \text{SIGN} \cdot \text{CAPLU})(2KU + 1)(KU + 1 - \text{SIGN} \cdot \text{CAPLU})}{2KU(KU + 1)}
\]

(20)

\[
S(R) = \frac{(KU + \text{SIGN} \cdot \text{CAPLU})(KU - 1 + \text{SIGN} \cdot \text{CAPLU})}{2KU}
\]

(21)

For \( \Delta \Lambda = +1 \) transitions (i.e., \( \Pi \rightarrow \Sigma, \Delta \rightarrow \Pi, \text{ etc.} \))

\[
\text{SIGN} = +1
\]

For \( \Delta \Lambda = -1 \) transitions (i.e., \( \Sigma \rightarrow \Pi, \Pi \rightarrow \Delta, \text{ etc.} \))

\[
\text{SIGN} = -1
\]

(c) Subroutine S2 PI2

The wave number \( (\text{NUBAR}) \) of each rotational line for these transitions (i.e., \( ^{2}\Sigma \leftrightarrow ^{2}\Pi \)) is defined by the equations in reference 9, page 232, or reference 7. In partial Fortran IV notation, the wave number is

\[
\text{NUBAR} = \text{NUBARO} + \text{BVU} \left[ (JU + 0.5)^2 - \text{CAPLU}^2 \right. \\
+ \frac{\text{SIGNU1}}{2} \sqrt{4(JU + 0.5)^2 - 4 \cdot \text{YU} \cdot \text{CAPLU}^2 + \left( \text{YU} \cdot \text{CAPLU} \right)^2} \\
- \text{BVU} \left[(JL + 0.5)^2 - \text{CAPLL}^2 \right. \\
+ \frac{\text{SIGNU2}}{2} \sqrt{4(JL + 0.5)^2 - 4 \cdot \text{YL} \cdot \text{CAPLL}^2 + \left( \text{YL} \cdot \text{CAPLL} \right)^2} \\
\left. \right]
\]

(22)

The line-strength expression for each branch (see ref. 11, or ref. 7) is given by one of the following general expressions

\[
S_1 = \frac{(2J + 1)^2 + \text{SIGNS1} \cdot (2J + 1) \cdot \text{U} \cdot (4J^2 + 4J + \text{CONST1} + 2Y \cdot \text{SIGNS2})}{16(J + \text{CONST2})}
\]

(23)
\[ S_2 = \frac{(2j+1)[(4j^2 + 4j - 1) - \text{SIGNSL}.U.(8j^3 + 12j^2 - 2j + \text{CONST3} + 2Y \cdot \text{SIGNS3})]}{16j(j + 1)} \]  

where

\[ U = [Y^2 - 4Y + (2j + 1)^2]^{-1/2} \]  

\[ J = J_U \text{ and } Y = Y_U = \text{CAPAU}/\text{BVU} \text{ for } ^2\Pi \rightarrow ^2\Sigma \text{ transitions} \]

\[ J = J_L \text{ and } Y = Y_L = \text{CAPAL}/\text{BVIL} \text{ for } ^2\Sigma \rightarrow ^2\Pi \text{ transitions} \]

The values of the constants in these expressions can be determined from references 9 and 11, and are tabulated in table I.

Integration in INTRVL and SLIT Subroutines

(a) Subroutine INTRVL

Subroutine INTRVL computes integrated intensities between the specified wavelengths \( \text{LAM1} \) and \( \text{LAM2} \). The integration is, simply,

\[ \text{TOTALI} = \int_{\text{LAM1}}^{\text{LAM2}} \text{ELAM} \cdot d\lambda \]  

A sketch to help clarify the notation used in the program is given in figure 6. The integration proceeds by assuming a linear variation of the spectral intensity between points in the array.

(b) Subroutine SLIT

Subroutine SLIT computes the output signal that would be recorded by an instrument measuring intensities equal to the computed spectrum. The instrument sensitivity is input by specifying the slit function and the absolute calibration. The slit function can be specified by a normalized Gaussian expression or by a series of linear segments. These two alternatives are illustrated in figure 7. In the case of a nonsymmetrical slit, as shown in figure 7(b), \( \text{LAMCL} \) is difficult to specify meaningfully. The width of the linear segment slit is defined as

\[ \text{WIDTH} = \int_{\text{RMIN}}^{\text{RMAX}} \text{RSLIT} \cdot d\lambda \]  

The instrument absolute calibration is input as a single factor, if the instrument is a fixed wavelength radiometer, and as a function of wavelength, if the instrument is a grating spectrograph or a scanning spectrometer (referred to hereafter as a scanning slit). A representative calibration curve (RIAM(M)) for a scanning slit is shown in figure 8.
The integration to yield the instrument output signal at a given wavelength is

\[
\text{SIGNAL} = \int \frac{\text{RSLIT} \cdot \text{RLAMCL} \cdot \text{ELAM}}{\text{C} \cdot \text{WIDTH}} \text{ d}\lambda
\]  

(28)

where RLAMCL is either the calibration factor for a fixed wavelength slit or the local value of the calibration function for a scanning slit and,

\[C = 1.0 \quad \text{for a linear-segment slit function}\]

\[C = 1.065 \quad \text{for a Gaussian slit function}\]

The integration at a given wavelength is illustrated in figure 9. For a scanning slit, the integration is performed repetitively at wavelength intervals given by STEP from LAMSL to LAMS2. Only 500 locations have been reserved in the computer for storing SIGNAL as a function of wavelength. However, after this storage is filled, the data are printed, permitting the storage to be used again for the next 500 points. Therefore, there is no limit to the number of instrument-output points that can be computed. The primary purpose of printing the data in 500 point blocks is to facilitate adding a machine-plotting option.

PROGRAM USAGE

The program is written in the Fortran IV computer language. It operates at Ames Research Center on an IBM 7094 computer as an overlay job, under the IBJOB Processor of the IBSYS Operating System, version 13.

A simplified flow chart of the main program, illustrating the step-by-step flow through the program, is shown in figure 1. The primary method used to control the sequence of operations is the presence or absence of data in various fields of certain data cards. The inset table in figure 1 lists the data cards that are tested and the data fields that are filled for each card type. Clearly, by testing for blanks (or zeros), the card type can be selected. At the end of each case, control is transferred back to the beginning of the program to read in the next case. There is no limit to the number of cases that can be "stacked."
## Deck Makeup

<table>
<thead>
<tr>
<th>Origin</th>
<th>Link</th>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>---</td>
<td>0</td>
<td>MAIN</td>
<td>Initializes factors for each case, directs logic to the appropriate subroutines, and solves the radiative-transport equation</td>
</tr>
<tr>
<td>---</td>
<td>0</td>
<td>BLOCK DATA</td>
<td>Fills array OUTPUT</td>
</tr>
<tr>
<td>---</td>
<td>0</td>
<td>SKIP</td>
<td>Positions data tape to start of desired file. User must provide this subroutine. (When called from SETUP it skips to the start of the next file, when called from VU VL it returns to the start of the present file.)</td>
</tr>
<tr>
<td>ALPHA</td>
<td>1</td>
<td>ILAMDA</td>
<td>Initializes the ILAM array with the specified incident radiation and initializes the EIAM array to 0.0</td>
</tr>
<tr>
<td>ALPHA</td>
<td>2</td>
<td>SETUP</td>
<td>Reads the molecular constants, computes the partition function, and determines the appropriate transition subroutine to generate the intensities</td>
</tr>
<tr>
<td>ALPHA</td>
<td>3</td>
<td>VU VL</td>
<td>Computes and reads vibrational band constants, determines the maximum rotational quantum number, and finds the intensity factor</td>
</tr>
<tr>
<td>ALPHA</td>
<td>4</td>
<td>ZERO</td>
<td>Computes parallel transitions for diatomic molecules</td>
</tr>
<tr>
<td>ALPHA</td>
<td>5</td>
<td>ONE</td>
<td>Computes perpendicular transitions for diatomic molecules</td>
</tr>
<tr>
<td>ALPHA</td>
<td>6</td>
<td>S2 PI2</td>
<td>Computes doublet sigma to doublet pi transitions (or vice versa) for diatomic molecules</td>
</tr>
<tr>
<td>ALPHA</td>
<td>7</td>
<td>ATOMIC</td>
<td>Computes the electronic transitions for atoms</td>
</tr>
<tr>
<td>ALPHA</td>
<td>8</td>
<td>PRINT</td>
<td>Tabulates spectral intensity vs. wavelength on the written output</td>
</tr>
<tr>
<td>ALPHA</td>
<td>9</td>
<td>INTRVL</td>
<td>Computes integrated intensities between specified wavelengths</td>
</tr>
<tr>
<td>ALPHA</td>
<td>10</td>
<td>SLIT</td>
<td>Computes the output signal given by a specified instrument sensitivity</td>
</tr>
<tr>
<td>ALPHA</td>
<td>11</td>
<td>GROWTH</td>
<td>Computes the curve-of-growth</td>
</tr>
</tbody>
</table>

### Tapes

<table>
<thead>
<tr>
<th>Logical tape number</th>
<th>Usage</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>Input</td>
</tr>
<tr>
<td>6</td>
<td>Output</td>
</tr>
<tr>
<td>9</td>
<td>Spectroscopic data tape. BCD format, 800 bits/inch.</td>
</tr>
</tbody>
</table>
Program Input

A complete description of all required data cards is given in appendix C. Clearly, for the program to function properly, a great many values must be specified correctly. To reduce the probability of costly human errors, the spectroscopic constants and Franck-Condon factors for 18 diatomic band systems are stored on magnetic tape. A listing of this tape is given in appendix D. The tape can be easily extended to include additional band systems.

The program logic is such that all spectroscopic constants for a given band system must be read from the tape, or all must be read from data cards. If the spectroscopic constants are read from the tape, then the Franck-Condon factors may also be read from the tape. However, because Franck-Condon factors are generally more uncertain than the spectroscopic constants, the option exists to override the Franck-Condon factor on the tape by specifying the desired value on the appropriate data card.

Computer Run Time

The time to run a single case on the computer is controlled primarily by the time required to generate the spontaneous-emission spectrum. Therefore, the computer run time can be estimated approximately by

\[ \text{Time} = c \cdot n \cdot \text{RANGE} \cdot \left( \frac{\text{WIDTHV}}{\text{DELLAM}} \right), \text{minutes} \] \hspace{1cm} (29)

where

- \( c \) constant found from experience with a given computer,
- \( \text{5.8} \times 10^{-5} \) minute/line for the ARC IBM 7094
- \( n \) total number of lines included in the computation

Error Flags

Tests are made at many strategic locations throughout the program to insure that obvious errors are not present in the data. If an obvious error is found, an appropriate statement is printed. If an error is found in the data for the externally incident radiation, the program skips to the next case. If an error is found in the data for a band system, the program transfers control to the PRINT subroutine, which prints, in tabular form, the spectrum computed to that point, and then skips to the next case. If an error is found in the data for a vibrational band, an appropriate statement is printed, and the band is omitted from the calculation. However, in this case, the solution will continue.
Sample Case

The sample case presented is intended to illustrate the general format of the printed output. Therefore, only a few of the program options are included. A complete checkout of all program options and error flag statements has been made, but such an extensive checkout does not seem appropriate for this report. The sample case selected for presentation is the CN(red) and atomic-nitrogen computation shown in figures 7(a) and 7(b) of reference 7. The printed output for this case is shown in appendix E. Considerable care has been taken to output all input data used in the computation and to clearly identify each of them. Standard spectroscopic nomenclature from reference 9 has been used where appropriate. Where this was not possible, more complete statements have been printed.

The heading on the printed output is composed of the information placed on the three title cards plus a statement of the spectral range of the computation and the wavelength interval between computation points. Following the heading, each molecular band system and atomic system specified is printed. The spectroscopic constants and thermodynamic conditions specified for each system are also printed, in addition to the computed values of the spontaneous-emission intensity.

The integrated intensity listed for each branch is the sum of the spontaneous emission from all rotational lines between KMIN and KMAX that fall within the spectral range of the computation. BAND TOTAL is simply the sum of the branch intensities. APPROXIMATE BAND TOTAL is computed by assuming that all the band radiation occurs at the band origin (see equation IV-74 on page 200 of reference 9) and is normally within 30 percent or less of the BAND TOTAL. A larger difference is shown here because most of the rotational lines fall outside the spectral range specified and, therefore, are not included in the BRANCH and BAND TOTAL values. After the vibrational bands specified for a band system have been computed, the integrated spontaneous emission from the entire system, SYSTEM TOTAL, is found by summing the BAND TOTAL values. In the sample case, only one band is specified so that SYSTEM TOTAL = BAND TOTAL. The output for the atomic-nitrogen lines illustrates a format similar to, but somewhat simpler than, that for the band systems. After the last molecular or atomic system has been completed, the sum of the integrated spontaneous emission from every rotational and atomic line that fell within the spectral range is printed.

Once the computation of the spontaneous-emission spectrum is complete, for a case or a layer, cards are read that specify whether an optically thin spectrum is desired, or whether the "true" spectrum given by the equation of radiative transfer is desired (see discussion in ref. 7). For this sample case, a "true" spectrum is specified for a radiating gas depth of 1.0 cm, and it is tabulated on the printed output. Only a partial tabulation is presented.

The final program option illustrated by this sample case is the spectrum as it would appear if recorded by a grating instrument. The slit function and spectral calibration assumed for the calculation are shown on the printed output, and in figure 7(b) of reference 7. The instrument sensitivity at any
wavelength is given by the product of these functions. The instrument output signal is found by integrating the product of the instrument sensitivity and the spectral intensity. A partial tabulation of the output signal as a function of wavelength is shown on the printed output, and can be compared with figure 7(a) of reference 7.

CONCLUDING REMARKS

The computer program presented is applicable, to some degree of approximation, to any "allowed" diatomic or atomic electronic transition. The program computes a "true" spectrum by using the equation of radiative transfer, which accounts for spontaneous emission, induced emission, absorption, and externally incident radiation. Considerable care has been taken to make the program easy to read and apply. Since standard spectroscopic notation is used and abundant comment statements are provided within the actual program listing, the user should be able to understand the program and not be forced to exhibit faith in a "canned" routine. In addition, the program was designed to enable additional subroutines to be added with only minor modifications to the main program. Likely candidates for addition to the program are subroutines to compute the free-free and free-bound continua.

Ames Research Center
National Aeronautics and Space Administration
124-07-01-15-00-21
APPENDIX A

LISTING OF PROGRAM STATEMENTS
C MAIN PROGRAM
C Initializes factors for each case, directs logic to the appropriate
C subroutines, and solves the radiative transport equation.

COMMON/CPLT/LAMMIN,LAMMAX,DELLAM,NARRAY,CINT3,FACTRI(5)
COMMON/CARRAY/ILAM(9000),ELAM(9000)
COMMON/CREAD/READI,READ2,READ3,READ4,READ5,READ6
COMMON/CBAND/ALPHA,U,BETA,U,CAPAL,CAPLU,DEU,DEZERU,REL_TERML
COMMON/CBAND2/WEU,WEYU,WEZU,WEZEL,WEYEL,DEUDEGENU,REL_TERML
COMMON/CEXTRA/INDEX,FILE,SYSTEM,TOTAL,OUTPUT(12)
DIMENSION TITLE(36)
REAL LAM,LAMMIN,LAMMAX,NUBARO,NUBARO,LUSPIN,LABMAD
LOGICAL NEWCAS

C READ THE FIRST CONTROL CARD IN EACH CASE. IF FIRST 4 COLUMNS DO NOT SPELL
C CASE, READ THROUGH TO THE NEXT CASE.
10 READ (5,505) SEARCH
IF (SEARCH .EQ. CASE) GO TO 20
GO TO 10
C INITIALIZE RUNNING SUMS, CONSTANTS, AND FLAGS FOR THE NEW CASE.
20 TOTAL=0,0
SYSTEM=0,0
DEPTH=0,0
CINTB=0,0
DO 30 M=1,5
FACTRI(M)=OUTPUT(I1)
NEWCAS=.FALSE.
C READ TITLE CARDS FOR THIS CASE,
READ(5,500) ITITLE(M),M=1,36
C PRINT TITLES ON WRITTEN OUTPUT,
WRITE(6,600) (TITLE(M),M=1,36)
C READ WAVELENGTH RANGE FOR CALCULATION AND WAVELENGTH INTERVAL BETWEEN
C POINTS IN THE COMPUTED SPECTRUM,
READ(5,501) LAMMIN,LAMMAX,DELLAM
C TEST DEllAM, IF IT IS TOO SMALL TO ALLOW COVERAGE FROM LAMMIN TO
C LAMMAX WITH 9,000 ENTRIES IN THE ARRAY, INCREASE DEllAM.
IF ((LAMMAX-LAMMIN)/DELLAM.GT.8999) DELLAM=(LAMMAX-LAMMIN)/8999
NARRAY=I.I+(LAMMAX-LAMMIN)/DELLAM
C ADJUST LAMMAX TO MAKE IT AN EVEN INCREMENT OF DEllAM AND WRITE GENERAL
C HEADING FOR THIS CASE.
ARRAY=NARRAY
LAMMAX=LAMMIN+(ARRAY-1.0)*DELLAM
WRITE(6,602) LAMMIN,LAMMAX,DELLAM
C SUBROUTINE ILAMDA Initializes the ILAM ARRAY WITH THE SPECIFIED
C INCIDENT RADIATION AND Initializes the ELAM ARRAY TO O.O.
C IF NEWCAS = .TRUE., AN ERROR WAS DETECTED IN THE INCIDENT SPECTRUM
C AND THIS CASE WILL BE OMITTED.
CALL (ILAMDA,NEWCAS)
IF (NEWCAS) GO TO 10
GO TO 50
C STATEMENT 40 IS A KEY READ STATEMENT IN THE PROGRAM. REQUIRED
C INFORMATION IS READ AND THE PROGRAM TESTS WHICH FIELDS HAVE DATA
C TO DETERMINE WHAT SHOULD BE DONE NEXT. WHEN RETURNING FROM THE
C ILAMDA OR ATOMIC SUBROUTINES, THIS CARD HAS ALREADY BEEN READ.
C THE FOLLOWING TABLE DEFINES THE FIELDS THAT ARE FILLED FOR
C EACH CARD TYPE.
C CARD TYPE READ1 READ2 READ3 READ4 READ5 READ6
C (COLUMNS) 1-10 11-20 21-30 31-40 41-45 51-55 61-65 66-72
C TYPE FIELD EIO.O EIO.O EIO.O EIO.O F5.0 A6
C VIBRATIONAL BAND VU VL KMIN KMAX
C BAND SYSTEM PARTCC TELECT TVIB TROT (INDEX) NAME
C ATOMIC SYSTEM ATOMCC TELECT PARTITION FUNCTION-Q NAME
C CURVE OF GROWTH LAM1 LAM2 GROWTH
C RADIATIVE TRANSPORT DEPTH LAYER
C PRINT SPECTRUM
C DONT PRINT SPECTRUM
C WHAT CARD TYPE HAS BEEN READ.
C IS THIS A VIBRATIONAL BAND.
50 IF (READ6 .EQ. BLANK) GO TO 70
C IS THIS A BAND SYSTEM.
IF (READ4 .NE. 0.0) GO TO 60
C IS THIS AN ATOMIC SYSTEM.
IF (READ3 .NE. 0.0) GO TO 110
C THE SPONTANEOUS EMISSION SPECTRUM FOR THIS CASE OR LAYER IS COMPLETE.
TOTAL=TOTAL+SYSTEM
IF (TOTAL .EQ. 0.0) GO TO 55
IF (SYSTEM .NE. 0.0) WRITE(6,606) SYSTEM, (FACTRI(M), M=1,5)
WRITE(6,607) TOTAL, (FACTRI(M), M=1,5)
SYSTEM=0.0 TOTAL=0.0
C IS THIS A CURVE OF GROWTH CALCULATION.
55 IF (READ2 .NE. 0.0) GO TO 115
C IS THIS A RADIATIVE TRANSPORT CALCULATION.
IF (READ1 .NE. 0.0) GO TO 120
GO TO 160
C TRANSFER CONTROL TO THE APPROPRIATE SUBROUTINE.
C SUBROUTINE SETUP READS THE MOLECULAR CONSTANTS, COMPUTES THE PARTITION
C FUNCTION, AND DETERMINES THE APPROPRIATE TRANSITION SUBROUTINE TO
C GENERATE INTENSITIES DUE TO SPONTANEOUS EMISSION. IF NEWCAS = .TRUE., AN ERROR
C WAS DETECTED IN THE MOLECULAR CONSTANTS AND THE REMAINDER OF THIS
C CASE WILL BE OMITTED.
60 CALL SETUP (NEWCAS)
IF (NEWCAS) GO TO 180
GO TO 40
C SUBROUTINE VU VL COMPUTES AND READS VIBRATIONAL BAND CONSTANTS
C AND DETERMINES THE MAXIMUM ROTATIONAL QUANTUM NUMBER AND THE INTENSITY
C FACTOR.
70 CALL VU VL (SKIPVV)
IF (SKIPVV .NE. 0.0) GO TO 40
GO TO (80,90,100), INDEX
C SUBROUTINE ZERO COMPUTES PARALLEL TRANSITIONS FOR DIATOMIC MOLECULES.
80 CALL ZERO
GO TO 40
C SUBROUTINE ONE COMPUTES PERPENDICULAR TRANSITIONS FOR
C DIATOMIC MOLECULES.
90 CALL ONE
GO TO 40
C SUBROUTINE S2 PI2 COMPUTES DOUBLET SIGMA TO DOUBLET PI TRANSITIONS
C (OR VICE VERSA) FOR DIATOMIC MOLECULES.
100 CALL S2PI2
GO TO 40
C SUBROUTINE ATOMIC COMPUTES ELECTRONIC TRANSITIONS FOR ATOMS.
110 CALL ATOMIC
GO TO 50
C THIS IS A CURVE-OF-GROWTH CALCULATION.
115 CALL GROWTH
DEPTH* 0.0
C RE-INITIALIZE THE ILAM ARRAY TO ENABLE A SEPARATE RADIATIVE TRANSPORT CALCULATION IF SPECIFIED.
DO 117 M=1,NARRAY
ILAM(M)=0.0
GO TO 40
C---------------------------------------------------------------
C THIS IS A RADIATIVE TRANSPORT SOLUTION. GENERATE THE ILAM ARRAY.
120 DEPTH =READI
WRITE(&tG08) DEPTH
DO 130 M=I_NARRAY
IF(ELAM(M) .LE. 1.0E-36) GO TO 130
COUNT=COUNT+1.0
LAMBDA=(LAMMIN +(COUNT-1.0)*DELAM)/DELLAM
BLAM1=1.0*EXP(-1.0*3879/(LAMBDATA*TELECT))/LAMBDATA**5
1
CILAM1=ALOG((1.0*EXP(-1.0*3879/(LAMBDATA*TELECT))))
1
1 CILAM2=ALOG(DLAMMIN)
CILAM3=ALOG(ELAM(M))
CILAM4=1.0*3879/(LAMBDATA*TELECT)+2.30259
COUNT=M
LAMBDA=(LAMMIN +(COUNT-1.0)*DELAM)/DELLAM
1
IF (CILAM4 .GT. 87.0) CILAM=M
CILAM4=EXP(CILAM4)
ILAM(M)=BLAM-(BLAM-ILAM(M))*EXP(-CILAM4)
130 CONTINUE
C THE ILAM ARRAY HAS BEEN GENERATED FOR THIS LAYER.
C INITIALIZE THE INTENSITY FACTOR AND ELAM ARRAY FOR THE NEXT LAYER,
CINT3=0.0
DO 140 M=1,NARRAY
140 FACTRI(M)= OUTPUT(F)
DO 150 M=1,NARRAY
150 ELAM(M)=0.0
GO TO 40
C---------------------------------------------------------------
C THE CALCULATION OF THE FINAL SPECTRAL INTENSITY ARRAY IS FINISHED.
C COMPLETE THE SOLUTION FOR THE OUTPUT OPTIONS DESIRED.
C IF THIS IS A RADIATIVE TRANSPORT SOLUTION, TRANSFER THE VALUES OF ILAM INTO THE ELAM ARRAY FOR CONVENIENCE IN LATER MANIPULATION.
160 IF(DEPTH .NE. 0.0) GO TO 180
DO 170 M=1,NARRAY
170 ELAM(M)=ILAM(M)
C GENERATE WAVELENGTHS AND STORE THEM IN THE ILAM ARRAY.
180 DO 190 M=1,NARRAY
CINT3=M
COUNT=COUNT+1.0
ILAM(M)=LAMMIN +(COUNT-1.0)*DELAM
190 CONTINUE
C IS THE SPECTRUM TO BE TABULATED.
IF(READ .NE. 0) CALL PRINT(INTRVL,NSLIT)
C SUBROUTINE PRINT TABULATES SPECTRAL INTENSITY VERSUS WAVELENGTH ON THE WRITTEN OUTPUT.
200 CALL PRINT(NAMESPACE)
IF (NAMESPACE) GO TO 210
C READ A CARD WHICH SPECIFIES THE NUMBER OF INTERVALS AND THE NUMBER OF SLITS TO BE CONSIDERED.
210 READ(SX5,503) NINTRVL,NSLIT
C SUBROUTINE INTRVL COMPUTES INTEGRATED INTENSITIES BETWEEN SPECIFIED WAVELENGTHS.
IF (NINTRVL .NE. 0) CALL INTRVL(NINTRVL)
C SUBROUTINE SLIT COMPUTES THE OUTPUT SIGNAL GIVEN BY A SPECIFIED INSTRUMENT SENSITIVITY.
IF (NSLIT .NE. 0) CALL SLIT(NSLIT)
GO TO 10
C---------------------------------------------------------------
C FORMATS FOR READ STATEMENTS.

26
500 FORMAT(12A6)
501 FORMAT(3E10.0)
502 FORMAT(6E10.0,21X,A6)
503 FORMAT(21X)
504 FORMAT(4E10.0)
505 FORMAT(1A4)

C FORMATS FOR WRITE STATEMENTS.
600 FORMAT(1HI) 29X I2A6/30X*12A6/30X I2A6)
601 FORMAT(I2A6)
602 FORMAT(/21X) 27HTHE SPECTRUM COMPUTED FROM .F8.2.4H TO .F8.2)
114H ANGSTROMS AT .F6.3) 19H ANGSTROM INTERVALS//)
606 FORMAT(/24X)73HTHIS IS A RADIATIVE TRANSPORT SOLUTION, DEPTH OF A
1Bove RADIATING LAYER IS .F9.3) 4H CM.//)
END

$IBFTC HFO75A

BLOCK DATA
C BLOCK DATA SUBROUTINE IS USED TO LOAD HOLLERITH INFORMATION INTO THE
C ARRAY, OUTPUT(I2). THIS ARRAY IS USED TO BUILD THE ARRAY FACTRI(5)
C FOR PRINTING THE INTENSITY FACTOR.
COMMON/CEXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUT(I2)
DATA (OUTPUT(M),M=I)I2,1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9,1
IH,1H-/
END

$IBFTC HFO75N

SUBROUTINE SKIPI(K)
C SUBROUTINE SKIPI POSITIONS THE SPECTROSCOPIC DATA TAPE (TAPE 9) TO THE
C PROPER FILE.
WRITE (6,700)
STOP
C FORMAT FOR ERROR STATEMENT.
700 FORMAT(/30X)48HTHE COMPUTATION WAS TERMINATED BECAUSE THE USER .
i23HHAS NOT SUPPLIED A SKIP/
230X)46HSUBROUTINE TO POSITION THE SPECTROSCOPIC DATA )
324HTAPE TO THE PROPER FILE.//)
END

$ORIGIN ALPHA
$IBFTC HFO75B

SUBROUTINE ILAMDA (NEWCAS)
C SUBROUTINE ILAMDA INITIALIZES THE ILAM ARRAY WITH THE SPECIFIED
C INCIDENT RADIATION AND INITIALIZES THE ELAM ARRAY TO 0.0.
COMMON/CPLT/LAMMIN,LAMMAX,DELLAM,NARRAY,CINT3,FACTRI(5)
COMMON/CARRAY/LAM1:9000),LAM2:9000)
COMMON/CREAD/READI,READ2,READ3,READ4,READ5,READ6
COMMON/CBAND/ALPHAU,BetaU,BETAU,CAPAU,CAPLU,CAPIL,DEL,DEZEROL,REU,TERMI/
1 ALPHAL,BETA,L,DELL,DEZEROM,RELM
COMMON/CBAND2/WEU.WEXEU,WEYEU,WEZEU,BVU,DVU,DEGENU,NU,ALTNAT
1 WEL.WEXEL,WELYEL,WEZEL,NVL
COMMON/CTEMP/TELECT,TROT
COMMON/CTH/TH/TH,L/PARTCC,NUBARO,O,AOE,CINTI,CINT2,KMIN,KNAX
COMMON/CEXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUT(I2)
REAL ILAM,LAMMAX,LAMMIN
LOGICAL NEWCAS
DATA BLANK/6H
C INITIALIZE VALUES SO THAT THE ILAM ARRAY CAN BE SET TO 0.0 IF AN INCIDENT
C SPECTRUM IS NOT SPECIFIED.
ELAM1=1.LAMMIN
ELAM2=LAMMAX
ELAM5=0
ELAM5=0
NLAM=1
NILAM=999
NOILAM= 0
C READ THE VALUES OF THE INCIDENT RADIATION VERSUS WAVELENGTH AND STORE
C THEM TEMPORARILY IN THE ILAM ARRAY.

27
READ(5,500) READ1, READ2, READ3, READ4, READ5, READ6

IF (READ6 .NE. BLANK) GO TO 20
NOILAM = 1
NLAM = NLAM + 2
ELAM(NLAM) = READ1
ELAM(NLAM+1) = READ2
ELAM(NLAM+2) = READ3
ELAM(NLAM+3) = READ4
GO TO 10

20 NLAM = NLAM + 1
IF (ELAM(NLAM) .EQ. 0.0) GO TO 25
M1 = 1
GO TO 50

25 NLAM = NLAM + 1
 IF (ELAM(NLAM) .GT. LAMMAX) GO TO 80
M1 = M1 + 1
GO TO 25

38 IF (M1 .EQ. 0) GO TO 80
DO 40 M = 2, NLAM
IF (ELAM(M) .LE. ELAM(M-1)) GO TO 80
40 CONTINUE

C INITIALIZE THE ILAM ARRAY.
DO 60 M = 1, NARRAY
ILAM(M) = ELAM(M1) + (ELAM(M1+1) - ELAM(M1)) * ILAMMIN + (M - M1) * DELLLAM / (ELAM(M1+1) - ELAM(M1))
60 IF (LAMMIN + M * DELLLAM .GT. ELAM(N1+1)) M1 = M1 + 1

C INITIALIZE THE ELAM ARRAY.
DO 70 M = 1, NARRAY
ELAM(M) = 0.0
70 CONTINUE

C THERE IS AN ERROR IN THE INCIDENT RADIATION DATA. WRITE
C AN ERROR MESSAGE AND Omit THIS CASE.
80 WRITE(6,700)
NEWCAS = .TRUE.
RETURN

C FORMATS FOR READ STATEMENTS.
500 FORMAT(4E10,0,FS,0_21X,A6)
C FORMATS FOR WRITE STATEMENTS.
600 FORMAT(4X,35HSPECTRAL INCIDENT ON GAS SAMPLE//
  1 51X,WAVELENGTH,10X,8HINTENSITY/
  2 51X,2HM,18X,9HINTENSITY/
  3 51X,SHANGSTROMS,15X,15HCM2-MICRON-SR//)
601 FORMAT(50X,F8.2,13X,1PE10.4)

C FORMAT FOR ERROR STATEMENT.
700 FORMAT(//22X,ONE OF THE FOLLOWING RESTRICTIONS ON THE INCIDENT
  1 37M SPECTRAL INTENSITY ARRAY WAS VIOLATED/
  2 39X,WAVELENGTH MUST BE LESS THAN OR EQUAL TO LAMMIN/
  3 39X,WAVELENGTHS MUST INCREASE MONOTONICALLY.
  4 39X,WAVELENGTH MUST BE LESS THAN OR EQUAL TO LAMMAX/
  5 39X,WAVELENGTHS MUST INCREASE MONOTONICALLY.
END
SUBROUTINE SETUP (NEWCAS)

C SUBROUTINE SETUP READS THE MOLECULAR CONSTANTS, COMPUTES THE PARTITION
C FUNCTION, AND DETERMINES THE APPROPRIATE TRANSITION SUBROUTINE TO
C GENERATE INTENSITIES DUE TO SPONTANEOUS EMISSION.

COMMON/CLOT/LAMMIN,LAMMAX,DELLAM,ARRAY,CINT1,FACTRI
COMMON/CLARR/LAM( 9000),ELAM( 9000)
COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
COMMON/CDBAND/WEL,WEX,WELY,WELWEL,WEZWEL,DELW,BLV,BLV
COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
COMMON/CBAND1/ALPHAU,BETAU,DEU,DZEROU,CAPAU,CAPLU
COMMON/CBAND2/WEU,WEXEU,WEYEU,WEZEU,DEGENU,TERMU
COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
COMMON/CTEMP/TELECT,TVIB,TROT
COMMON/CWIDTH/WIDTHL,WIDTV,WIDTV,TERM
COMMON/CXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUT(12)

DIMENSION ALPHA(30),BETA(30),DEGEN(30),TERM(M2),WE(M2),WEXE(M2),WEYE(M2)

REAL KMAX1,KMAX2
LOGICAL NEWCAS

DATA ENDS/'END', BLANK/'BLANK', STATE/'STATE', ODD/'ODD', EVEN/'EVEN'
REWIND 9

C A NEW BAND SYSTEM HAS BEEN SPECIFIED.
PARTCC=READ1
TELECT=READ2
TVIB=READ3
TROT=READ4
INDEX=READ5+C

C WRITE THE INTEGRATED INTENSITY DUE TO SPONTANEOUS EMISSION FOR THE
C PREVIOUSLY COMPUTED SYSTEM.
IF (SYSTEM .NE. O.O) WRITE(6,600) SYSTEM,(FACTRI(M),M=1,5)
TOTAL=TOTAL+SYSTEM
SYSTEM=O.O

C ARE THE CONSTANTS FOR THIS BAND SYSTEM INPUT ON CARDS.
IF (INDEX .NE. O) GO TO 40
C THE CONSTANTS FOR THIS BAND SYSTEM ARE ON TAPE.
10 READ(9,900) NAME, INDEX, NFILE
IF (NAME .EQ. ENDS) GO TO 120
IF (NAME .EQ. READ6) GO TO 20
CALL SKIP(I,9)
GO TO 10

C READ PAST THE FRANCK-CONDON FACTORS, USING TERM(M2) AS A DUMMY
C ARRAY.
20 DO 30 M2=1,20
30 READ(9,901) (TERM(M2), M2=1,20)
C READ THE CONSTANTS FROM TAPE.
READ(9,902) READ1,ALTNAT,DEU,BETAU,REU,DZEROU,CAPAU,CAPLU
READ(9,902) MU,NUSPIN,DEL,BETAU,REU,DZEROU,CAPAU,CAPLU
READ(9,902) LEVELS=READ1(+1)
READ(9,902) (DEGEN(M),TERM(M),WE(M),WEXE(M),WEYE(M),WEZEU(M),BE(M)
1 +ALPHA(M),M=1,LEVELS)
GO TO 50

C ARE THE CONSTANTS FOR THIS BAND SYSTEM TO BE INPUT ON CARDS.
40 READ(5,500) READ1,ALTNAT,DEU,BETAU,REU,DZEROU,CAPAU,CAPLU
READ(5,500) MU,NUSPIN,DEL,BETAU,REU,DZEROU,CAPAU,CAPLU
READ(5,500) LEVELS=READ1(+1)
READ(5,500) (DEGEN(M),TERM(M),WE(M),WEXE(M),WEYE(M),BE(M)
1 +ALPHA(M),M=1,LEVELS)
NFILE= 0

C STORE UPPER AND LOWER STATE SPECTROSCOPIC CONSTANTS FOR THIS SYSTEM.
50 ALPHA=ALPHA(1)
ALPHA=ALPHA(2)
DEU=DE(1)
BETAU=B(2)
DEGENU=DEGENU
TERMU=TERM(1)
TERM=TERM(2)
WEL=WEL(1)
WEL=WEL(2)
WEX=WEX(1)
WEX=WEX(2)
WEYE=WYE(1)
WEYE=WYE(2)
WEZE=WZE(1)
WEZE=WZE(2)
C FIND Q, THE PARTITION FUNCTION REFERENCED TO THE EQUILIBRIUM POSITION
C OF THE GROUND STATE POTENTIAL WELL

Q=0.0
GO TO M=1.LEVELS
QVR=0.0
QV=0.0
EVIB1=0.0
V=0.0
60 EVIB2=WE(M)*(V+0.5) -WEEXE(M)*(V+0.5)**2 +WEYE(M)*(V+0.5)**3
+WEZE(M)*(V+0.5)**4
DELTQV=EXP(-1.43879*EVIB2/EVIB2)
C COMPARE DELTA Q-VIBRATIONAL TO 0.1 PERCENT OF THE QV SUM TO THIS
C POINT:
IF (DELTQV .LE. 0.001*QV) GO TO 70
C HAS THE VIBRATIONAL ENERGY REACHED A FICTITIOUS PEAK?
IF (EVIB2 .LE. EVIB1) GO TO 70
Q=Q+DELTQV
QVR=QVR+TROT_DELTQV/(1.43879*(BE(M)-ALPHA(M)**0.5))
EVIB2=EVIB2
V=V+1.0
GO TO 60
70 Q=Q*DEGEN(M)*EXP(-1.43879*TERM(M)/TELECT)
C WRITE THE INPUT DATA FOR THE NEW SYSTEM.
WRITE(6,601) READ6,PARCC,TELECT,TWIB,TROT
WRITE(6,602) ALTNT,NUSPIN,LEVELS,ALPH
ICAPLU= ICAPLU+1
ICAPLL= ICAPLL+1
WRITE(6,603) ICAPLU,ICAPLL,DEGEN(M),EVIB1,NE,NEE
WRITE(6,604) ICAPLU,ICAPLL,DEGEN(M),EVIB1,NE,NEE
DO 100 M=1.LEVELS
DUMMY(1)=BLANK
DUMMY(2)=BLANK
IF (M .NE. 1) GO TO 80
DUMMY(1)= UPPER
DUMMY(2)= STATE
80 IF (M .NE. 2) GO TO 90
DUMMY(1)= LOWER
DUMMY(2)= STATE
90 MDUMMY = DEGEN(M)
100 WRITE(6,605) DUMMY(1),DUMMY(2),MDUMMY,TERM(M),WE(M),WEEXE(M),
+WEYE(M),WEZE(M),BE(M),ALPHA(M)
C IF LINES ALTERNATE IN INTENSITY, WRITE OUT RATIO OF INTENSITIES.
IF (ALTNT .EQ. 0.0) GO TO 110
DUMMY1=0.DO
IF (ALTNT .EQ. 2.DO) DUMMY1=1.DO
RATIO=NUSPIN/NUSPIN+1.0
WRITE(6,606) DUMMY1,RATIO
C IS THE UPPER ELECTRONIC TERM ENERGY GREATER THAN THE LOWER ELECTRONIC
C TERM ENERGY? IF NOT, WRITE AN ERROR MESSAGE AND OMIT THIS CASE.
110 IF (TERMU .LE. TERML) GO TO 130
C WRITE THE OUTPUT HEADING FOR VIBRATIONAL BANDS.
WRITE(6,607)
RETURN
C THERE IS AN ERROR IN THE BAND SYSTEM NAME. WRITE AN ERROR MESSAGE
C AND OMIT THIS CASE.
120 WRITE(6,700) READ6
GO TO 140
C THERE IS AN ERROR IN THE TERM ENERGIES. WRITE AN ERROR MESSAGE AND
C OMIT THIS CASE.
130 WRITE(6,701)
140 NEWCAS=.TRUE.
RETURN
C FORMATS FOR READ STATEMENTS.
500 FORMAT(8E10.0)
501 FORMAT(4E10.0,F5.0,21X,A6)
502 FORMAT(215)
C FORMATS FOR WRITE STATEMENTS.
600 FORMAT(/102X,SYSTEM TOTAL,2X,IPeleo,4.5A1)
601 FORMAT(/65X,AD/)
 1 21X,12HTOTAL NUMBER,13X,10HELECTRONIC,14X,11HVIBRATIONAL,13X,
 2 10HROTATIONAL/,
 3 21X,12HOF MOLECULES,313X,11HTEMPERATURE/,
 4 21X,7HPER CC,9X,3115X,9HDEGREES K/,
 5 21X,1PE10.4,1X,3114X,11OE3,31/
SUBROUTINE VU VL (SKIPVV)
C SUBROUTINE VU VL COMPUTES AND READS VIBRATIONAL BAND CONSTANTS
C AND DETERMINES THE MAXIMUM ROTATIONAL QUANTUM NUMBER AND THE INTENSITY
C FACTOR.
COMMON/CPLOT/LAMMIN,LAMMAX,DELAM,NARRAY,CINT3_FACTRI(15)
COMMON/CARRAY/ILAM(9000),ELAM(9000)
COMMON/CREAD/READI,READ2,READ3,READ4,READS,READ6
COMMON/CBAND1/ALPHAU,BETAU,CAPAU,CAPLU,DEU,DZEROU,REU_TERMU,
  ALPHA,BETAL,CAPAL,CAPLL,DEL,DZEROL,REL_TERML
COMMON/CBAND2/WEU,WEXEU,WEYE,WEZE,BVU,DVU_DEGENU,MU,ALTNAT,
  WEL,WEXEL,WEYEL,WEZEL,BVL,DVL_USPIN
COMMON/CTEMP/TELECT,TVIB,TROT
COMMON/CM/WIDTH/1000,WIDTH/RANGE
COMMON/CTBAR/PARTIC,KBARADO,Q,ADE,CINT1,CINT2,KMIN+KMAX
COMMON/CEXTRA/INDEX,FILE,SYSTEM,TOTAL,OUTPUT(12)
REAL MU,KMAX2,KMAX1,NUBARO,LOWER,ILAM_NAME
DIMENSION QVV(20)
INTEGER FLAG
DATA UPPER/6HUPPER/, LOWER/6HLOWER/
SKIPVV= 0,0
AOE=2,54E18
C=2,9979E+10
PI=3,1415927
VU=READI
VL=READ2
KMIN=READ3
KMAX=READ4
C TEST VIBRATIONAL QUANTUM NUMBERS TO ENSURE THAT FICTITIOUS PEAK
C VIBRATIONAL TERM ENERGY OF THE UPPER STATE IS LESS THAN OR EQUAL TO THE TERM ENERGY OF THE LOWER STATE.
C FORMATS FOR ERROR STATEMENTS.
700 FORMAT///10X,3HTHE,1X,A6,12H BAND SYSTEM,2OH IS NOT ON THE TAPE.)
701 FORMAT///10X,12HHERREN = ELECTRONIC TERM ENERGY OF THE UPPER STATE
C FORMATS FOR TAPE READ STATEMENTS.
900 FORMAT(A6,216)
901 FORMAT(S14,T)
902 FORMAT(BE14.?)
END
S$ORIGIN ALPHA
$1BFTC HF05D0
C SUBROUTINE VU VL COMPUTES AND READS VIBRATIONAL BAND CONSTANTS
C AND DETERMINES THE MAXIMUM ROTATIONAL QUANTUM NUMBER AND THE INTENSITY
C FACTOR.
COMMON/CPLOT/LAMMIN,LAMMAX,DELAM,NARRAY,CINT3_FACTRI(15)
COMMON/CARRAY/ILAM(9000),ELAM(9000)
COMMON/CREAD/READI,READ2,READ3,READ4,READS,READ6
COMMON/CBAND1/ALPHAU,BETAU,CAPAU,CAPLU,DEU,DZEROU,REU_TERMU,
  ALPHA,BETAL,CAPAL,CAPLL,DEL,DZEROL,REL_TERML
COMMON/CBAND2/WEU,WEXEU,WEYE,WEZE,BVU,DVU_DEGENU,MU,ALTNAT,
  WEL,WEXEL,WEYEL,WEZEL,BVL,DVL_USPIN
COMMON/CTEMP/TELECT,TVIB,TROT
COMMON/CM/WIDTH/1000,WIDTH/RANGE
COMMON/CTBAR/PARTIC,KBARADO,Q,ADE,CINT1,CINT2,KMIN+KMAX
COMMON/CEXTRA/INDEX,FILE,SYSTEM,TOTAL,OUTPUT(12)
REAL MU,KMAX2,KMAX1,NUBARO,LOWER,ILAM_NAME
DIMENSION QVV(20)
INTEGER FLAG
DATA UPPER/6HUPPER/, LOWER/6HLOWER/
SKIPVV= 0,0
AOE=2,54E18
C=2,9979E+10
PI=3,1415927
VU=READI
VL=READ2
KMIN=READ3
KMAX=READ4
C TEST VIBRATIONAL QUANTUM NUMBERS TO ENSURE THAT FICTITIOUS PEAK
C VIBRATIONAL TERM ENERGY OF THE UPPER STATE IS LESS THAN OR EQUAL TO THE TERM ENERGY OF THE LOWER STATE.
C FORMATS FOR ERROR STATEMENTS.
700 FORMAT///10X,3HTHE,1X,A6,12H BAND SYSTEM,2OH IS NOT ON THE TAPE.)
701 FORMAT///10X,12HHERREN = ELECTRONIC TERM ENERGY OF THE UPPER STATE
C FORMATS FOR TAPE READ STATEMENTS.
900 FORMAT(A6,216)
901 FORMAT(S14,T)
902 FORMAT(BE14.?)
END
C LOWER STATE.
5 WE = WEL
WEEX = WEXEL
WEY = WEYEL
WEZE = WEZEL
MV = VL + 1
10 EVI = 0
FLAG = FLAG + 1
DO 20 M = I, MV
V = M - 1
EV2 = WE(V + 0.5) - WEEX(V + 0.5)**2 - WEY(V + 0.5)**3 - WEZE(V + 0.5)**4
IF(EV2 > EVI) GO TO 230
20 EVI = EV2
IF(FLAG.EQ.1) GO TO 5

C COMPUTE ROTATIONAL CONSTANTS FOR THIS BAND.
30 BVU=BEU-ALPHAU*(VU+0.5)
BVL=BEL-ALPHAL*(VL+0.5)
DVU=DEU+BETAU*(VU+0.5)
DVL=DEL+BETAL*(VL+0.5)

C READ VIBRATIONAL BAND CONSTANTS.
READ(5,500) SUMRE2,WIDTHG,WIDTHL,NUBAR0,FRANCK,RANGE
C IF A FRANCK-CONDON FACTOR WAS READ, CONTINUE WITH
C THE SOLUTION. IF ONE WAS NOT READ AND THE MOLECULAR AND SPECTROSCOPIC
C CONSTANTS WERE NOT READ FROM TAPE, THEN THE SOLUTION CANNOT PROCEED.
IF (FRANCK .GT. 0.0) GO TO 40
IF (NFILE .EQ. 0) GO TO 240
C READ FRANCK-CONDON FACTORS FROM TAPE USING THE WEZE ARRAY FOR
C TEMPORARY STORAGE.
CALL SKIP(-0,0)
READ(9,900) NAME, INDEX, NFILE
NI=VU+1
N2=VL+1
READ(9,901) ((QVV(M2), M2=I,20), M1:I, NI)
FRANCK=QVV(N2)
C RANGE IS THE DISTANCE FROM THE LINE CENTER, IN LINE WIDTHS, BEYOND
C WHICH THE SPONTANEOUS LINE EMISSION IS CONSIDERED ZERO.
40 IF(RANGE .NE. 0.0) GO TO 45
IF (WIDTHL .EQ. 0.0) RANGE=3.0
C FIND THE VOIGT LINE WIDTH AT HALF-HEIGHT. IF LINE WIDTHS WERE NOT INPUT
C IMPOSE A GAUSSIAN PROFILE WITH A WIDTH TEN TIMES DELLAM.
45 WIDTHV=WIDTHL/2.0+SQRT(WIDTHL**2/4.0+WIDTHG**2)
IF (WIDTHV .NE. 0.0) GO TO 50
WIDTHV=10.0*DELLAM
WIDTHV=WIDTHV
WRITE(6,701)
C FIND KMAX, THE MAXIMUM ROTATIONAL QUANTUM NUMBER POSSIBLE FOR THE
C SPECIFIED VIBRATIONAL LEVELS. KMAX VALUES ARE FOUND FOR BOTH THE
C UPPER AND LOWER STATES. HOWEVER, VALUE OF THE KMAX USED BY THE PROGRAM
C IS THE MINIMUM OF THESE AND THE INPUT VALUE IF IT IS NOT ZERO. IF THE
C DISSOCIATION ENERGY IS NOT INPUT, KMAX CANNOT BE DETERMINED AND IS SET TO
C THE INPUT VALUE OR 150 IF THE INPUT VALUE IS ZERO.
C SEE HERZBERG, PAGE 426, FOR A DISCUSSION OF DISSOCIATION DUE TO ROTATION.
C SET UP CONSTANTS TO FIND KMAX FOR LOWER STATE.
50 IF (DZERO < 0.0) GO TO 60
DEQUEL=DZERO + WEL/2.0 - WEEXL/4.0 + WEYL/8.0 + WEZEL/16.0
EVIRL=WEL*(VL+0.5) - WEEXL*(VL+0.5)**2 + WEYL*(VL+0.5)**3 + WEZEL*(VL+0.5)**4
C1=1.2177E7*WEL*SQRT(MU/DEQUEL)
REQL=REK
DV=HVL
BV=HVL
GO TO 70
C SET UP CONSTANTS TO FIND KMAX FOR UPPER STATE.
60 IF (DZERO < 0.0) GO TO 170
DEQUEL=DZERO + WEU/2.0 - WEUE/4.0 + WEUEL/8.0 + WEZEU/16.0
EVIRUE=WEU*(VU+0.5) - WEUEL*(VU+0.5)**2 + WEUEL*(VU+0.5)**3 + WEZEU*(VU+0.5)**4
C1=1.2177E7*WEEL*SQRT(MU/DEQUEL)
REQL=REU
DV=HVU
BV=HVU
C IF VIBRATIONAL ENERGY IS GREATER THAN OR EQUAL TO THE DISSOCIATION
C ENERGY, THIS BAND CANNOT EXIST.
70 IF (EVIRB >= DEQUEL) GO TO 220
C SET THE INITIAL VALUES NEEDED TO START THE ITERATION.
C KMAX1 = PRIOR VALUE OF KMAX
C KMAX2 = PRESENT VALUE OF KMAX
C KMAX3 = INTEGER VALUE OF NEXT KMAX
C K = INTEGER VALUE OF KMAX2
C E1 AND E2 = PRIOR AND PRESENT SUMS OF VIBRATIONAL PLUS ROTATIONAL ENERGY
C U1 AND U2 = PRIOR AND PRESENT VALUES OF EFFECTIVE POTENTIAL ENERGY AT THE
C LOCAL MAXIMUM.
C FLAG=1 INDICATES THIS IS THE FIRST ITERATION.

C3=1.668E-15/MU
E1=EVIB
U1=DEQUIL
KMAX1=0.0
K=50
KMAX2=K
FLAG=1

C FIND R, THE INTERNUCLEAR DISTANCE AT THE LOCAL MAXIMUM OF THE
C EFFECTIVE POTENTIAL WELL FOR KMNX2. A MORSE CURVE IS ASSUMED
C FOR THE POTENTIAL WELL WITHOUT ROTATION.

80 R=REQUIL
FR2=0.0
FK=C3*1.0E+24*KMAX2*(KMAX2+1.0)/RI_OEQUIL)

90 FR1=FR2
R=R+0.1E-8
IF (R.GT.1.0E-7) GO TO 120
C2=EXP(-C1*(R-REQUIL))
FR2=FR2+1.0E+8*EXP(-C1*R)
IF (FR2.GT.FR1) GO TO 90
IF (FR1.GT.FK) GO TO 110
IF (FR1.EQ.FR2) GO TO 100

C A LOCAL MAXIMUM DOES NOT EXIST AT K.
C SET R TO PRIOR VALUE AND CONTINUE ITERATION.
R=R-0.1E-8
GO TO 120

C THE LOCAL MAXIMUM AT K IS, IN FACT, A CRITICAL POINT.
C SET R TO CRITICAL POINT AND CONTINUE ITERATION.

100 R=R-0.1E-8
GO TO 120

C INTERPOLATE TO GET VALUE OF R AT LOCAL MAXIMUM.

110 R=R-0.1E-8*(FK-FR2)/(FR1-FR2)
C FIND THE NEXT VALUE OF KMAX (I.E., KMAX3) DURING THE FIRST ITERATION
C STEP KMAX2 BY 20 UNTIL U2 IS LESS THAN OR EQUAL TO E2 AND THEN
C INTERPOLATE TO U=E TO GET KMAX3. IN ALL OTHER ITERATIONS, JUST
C EXTRAPOLATE TO U=E TO GET KMAX3.

120 E2=EVIB +BV*KMAX2*(KMAX2+1.0) -DV*KMAX2**2*(KMAX2+1.0)**2
U2=DEQUIL*(1.0-EXP(-C1*(R-REQUIL)))*C3*KMAX2*(KMAX2+1.0)/R**2
IF (FLAG .NE. 1) GO TO 140
IF (U2 .LE. E2) GO TO 130
KMAX3=KMAX2
KMAX2=KMAX3+20.0
K=KMAX2+0.1
IF (KMAX2 .GE. 500.0) GO TO 150
E1=E2
U1=U2
GO TO 80

130 FLAG=2
140 KMAX3=KMAX2 +((U2-E2)*(KMAX2-KMAX1)/(U2-E1)-(U2-E2))
C IF KMAX3 IS LESS THAN OR EQUAL TO ZERO, THIS VIBRATIONAL LEVEL
C CANNOT EXIST.
IF (KMAX3 .LE. 0) GO TO 260
C WHEN KMAX3 EQUALS K, THE ITERATION IS COMPLETE.
IF (KMAX3 .EQ. K) GO TO 160
E=KMAX3
KMAX1=KMAX2
KMAX2=KMAX3
E1=E2
U1=U2
GO TO 80

150 KMAX3=KMAX2+0.1
C THE ITERATION IS COMPLETE. SET KMAX.

160 IF (KMAX .EQ. 0) KMAX=KMAX3
IF (KMAX .LT. KMAX) KMAX=KMAX3
IF (BV .EQ. 0.0) GO TO 80
IF (KMAX .EQ. 0) KMAX=150
C SET UP CONSTANTS FOR INTENSITY EQUATION IN ROTATIONAL STRUCTURE
C SUBROUTINE AND COMPUTE NUBARO, THE BAND ORIGIN, IF NOT SPECIFIED.
C
CINT1=TERMU/TELECT +WEU*(VU+0.5)-WEXEU*(VU+0.5)**2+WEYEU*
( VU+0.5)**3+WEZEU*(VU+0.5)**4)/TVIB
CINT2=(16.0E-7*PARTCC*FRANCK*SUMRE2*PIW**3)/(3.0E0)
IF (NUBARO .EQ. 0.0) NUBARO=TERMU -TERML +WEU*(VU+0.5) -WEXEU*
1*(VU+0.5)**2 +WEYEU*(VU+0.5)**3+WEZEU*(VU+0.5)**4 -WEL*(VL+0.5)**2
3+WEYEL*(VL+0.5)**3 -WEZEL*(VL+0.5)**4
ORIGIN=1.0E+8/NUBARO
C FIND THE INTENSITY FACTOR, IF NECESSARY.
IFACTR= 0.62486*CINT1
IF(IFACTR .LT. 30.0) GO TO 210
CINT4=IFACTR
IF(CINT4 .LT. CINT3) GO TO 210
FACTRI(1)=OUTPUT(12)
DO 180 M1=295
FACTRI(M1)=OUTPUT(M1)
IFACTR=IFACTR-M1*IO*W(5-M1)
180 M=IFACTR/IOWW(4-M1)
C IF THIS IS NOT THE FIRST INTENSITY FACTOR, ADJUST THE ELAM ARRAY.
IF(CINT3 .EQ. 0.0) GO TO 200
CINT|= CINT= CINT3
DO 190 M1=1,NARRAY
190 ELAM(M1)=ELAM(M1)*EXP(2.30259*CINT5)
SYSTEM= SYSTEM*EXP(2.30259*CINT5)
TOTAL= TOTAL*EXP(2.30259*CINT5)
200 CINT3= CINT4
C WRITE THE VIBRATIONAL BAND INFORMATION.
210 MI=VU+ 0.1
M2=VL+ 0.1
IRANGE= RANGE+ 0.1
IF(KMIN .LT. 2) KMIN= 2
WRITE(*,600)MI,M2,FRANCK,SUMRE2,WIDTHG,WIDTHL,WIDTHV,IRANGE,
1 ORIGIN,KMIN,KMAX
IF (CINT2 .LE. 0.0) GO TO 250
RETURN
C THIS VIBRATIONAL LEVEL CANNOT EXIST, WRITE THE APPROPRIATE MESSAGE
C AND OMIT THIS BAND.
220 MI=VU+ 0.1
M2=VL+ 0.1
DUMMY=UPPER
IF (WE .EQ. WEL) DUMMY=LOWER
WRITE(*,702) MI,M2,DUMMY
SKIPVV= 1.0
RETURN
230 MI=VU+ 0.1
M2=VL+ 0.1
DUMMY=UPPER
IF (WE .EQ. WEL) DUMMY=LOWER
WRITE(*,705) MI,M2,DUMMY
READ(5,500) SUMRE2,WIDTHG,WIDTHL,NUBARO,FRANCK,RANGE
SKIPVV= 1.0
RETURN
C THERE IS AN ERROR IN THE FRANCK-CONDON FACTOR, WRITE AN ERROR MESSAGE
C AND OMIT THIS BAND.
240 MI=VU+ 0.1
M2=VL+ 0.1
WRITE(*,703) MI,M2
SKIPVV= 1.0
RETURN
C THE BAND INTENSITY IS ZERO DUE TO A POSSIBLE ERROR IN PARTCC, FRANCK, SUMRE2,
C OR Q, WRITE THE APPROPRIATE MESSAGE AND OMIT THIS BAND.
250 WRITE(*,700)
SKIPVV= 1.0
RETURN
C THE MAX POSSIBLE ROTATIONAL QUANTUM NUMBER IS LESS THAN OR EQUAL
C TO ZERO, WRITE THE APPROPRIATE MESSAGE AND OMIT THIS BAND.
260 MI=VU+ 0.1
M2=VL+ 0.1
WRITE(*,706) MI,M2
SKIPVV= 1.0
RETURN
C FORMAT FOR READ STATEMENT.
C FORMAT FOR WRITE STATEMENT.

600 FORMAT(/IX,12,4X,12,6X,IPE10.4,3X,E10.4,9X,3(0F9.4,1X))
700 FORMAT(/4X,12,6X,IPE10.4,3X,E10.4,9X,3(OPF9.4,1X)'3X'I4,

C FORMATS FOR ERROR STATEMENTS.

702 FORMAT(/4X,12,6X,IPE10.4,3X,E10.4,9X,3(OPF9.4,1X)'3X'I4,

C FORMATS FOR THE TAPE STATEMENTS.

900 FORMAT(A6,2I6)
901 FORMAT(SEI4.7)

END

$ORIGIN ALPHA
$IBFTC HF075E

SUBROUTINE ZERO

C SUBROUTINE ZERO COMPUTES PARALLEL TRANSITIONS FOR DIATOMIC MOLECULES.

COMMON/CPLLOT/LAMMIN,LAMMAX,DELLAM,NARRAY,CINT3 FACTRI(5)
COMMON/CARRAY/ILAM(9000),ELAM(9000)
COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
COMMON/CRAND/ALPHAU,BETAU,CAPAU,CAPLU,DEU,DZEROU,REU,TERMU,
ALPHAL,BETAL,CAPAL,CAPLL,DELL,BELL,RELL,TERMLL
COMMON/CBAND1/WEU,WEXEU,WEYEU,WEZEU,BVEL,BVLL,WELOGU,WELOGL,ALTU,
WELOGE,ALTLL,WELOGR,ALTLL,WELOGF,ALTLL,WELOGG,ALTLL
COMMON/CBAND2/WEU,WEXEU,WEYEU,WEZEU,BVEL,BVLL,WELOGU,WELOGL,ALTU,
WELOGE,ALTLL,WELOGR,ALTLL,WELOGF,ALTLL,WELOGG,ALTLL
COMMON/CTEMP/TELECT,TVIB,TROT
COMMON/CTRAN/PARTCC,NUBARO_Q,AOE,CINT1,CINT2,KMIN,KMAX
COMMON/CEXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUT(12)

REAL ILAM,KU,KL,LAMCL,LAMBDA_LAMMAX,LAMMIN,NUBAR,NUBARO,NUSPIN

C FIND THE NUMBER OF ENTRIES IN THE INTENSITY ARRAY, FROM THE LINE CLUSTER.
C AT WHICH EACH LINE IS ASSUMED TO HAVE A CONTRIBUTION.

NSPRED=1.1+RANGE*WIDTHV/DELLAM

C SET CONSTANTS WHICH DETERMINE THE LINE SHAPE.

CSPRD2=WIDTHV/WIDTHL
CSPRD3=(1.050+0.447*CSPRD2*0.058*CSPRD2**2)*WIDTHV*1.0E-4
CSPRD1=(1.10-CSPRD2)**2
CSPRD2=1.0+0.5*CSPRD1

C SET CONSTANTS WHICH DETERMINE THE WAVELENGTH OF THE LINE CENTER FOR
C TRIPLETS. SEE HERZBERG, PAGE 235.

YUE=CAPAU/BVEL
YL=CAPAL/BVLL

DIVISR=2.0
IF (CAPLU .EQ. 0.0) DIVISR=1.0

C SET CONSTANTS FOR THE P BRANCH AND INITIALIZE THE RUNNING SUMS.

CSTRI=1.0
KUKMIN=1.0
KLU=1.0
KLL=0.0
BAND=0.0

10 BRANCH=0.0

C COMPUTE AND DISTRIBUTE THE INTEGRATED INTENSITY DUE TO SPONTANEOUS
C EMISSION OF ALL SPECIFIED ROTATIONAL LINES.

DO 60 I=KMIN,KMAX
2NU=0.0
2NL=0.0

C FOR A DESCRIPTION OF THESE EQUATIONS, SEE HERZBERG, PAGE 235.

IF (OGENEU/DIVISR+NE+3.0) GO TO 20
ZIU=CAPU**2*YU**4+DZERU**2*4.0*YU+4.0*YU**2+4.0*KU**2
ZIL=CAPL**2*YU**4+DZERL**2*4.0*YU+4.0*KL**2
ZIU4=CAPU**2*KYU**4+4.0*KYU**2+4.0*KU**2+4.0*KU**2
ZIL4=CAPL**2*KYU**4+4.0*KYU**2+4.0*KL**2+4.0*KL**2
2NU=ADDU+ADDL
2NL=ADDL+ADDL

20 CONTINUE
C COMPUTE THE WAVELENGTH OF THE LINE CENTER IN ANGSTROMS.

20  NUBAR=NUBARO +B(VU*(KU-KU+1,0)+4,0)*ZU1 -B(VU*(KL+1,0)+4,0)*ZL1 -DVU*(KU+0,5)**4 +DVU*(KL+0,5)**4
    LAMCL=1,0*E/NUBAR
C IF THE LINE WAVELENGTH FALLS OUTSIDE THE SPECTRAL RANGE OF
C INTEREST, OMIT IT AND PROCEED TO THE NEXT LINE.
    IF(LAMCL.LT.LAMMIN-RANGE*WIDTHV) GO TO 50
    IF(LAMCL.GT.LAMMAX+RANGE*WIDTHV) GO TO 50
C FIND THE STRENGTH FACTOR.
    S=KU+CSTR
C DETERMINE IF LINES ALTERNATE IN INTENSITY.
    FACTRI=1,0
    IF(ALTNAT .EQ. 0,0) GO TO 30
C EVALUATE THE ALTERNATION FACTOR FOR HOMONUCLEAR MOLECULES.
C THE EXPONENT IN THE ALTERNATING FUNCTION IS FOUND SEPARATELY TO ENSURE
C THAT IT IS AN INTEGER BEFORE RAISING (-1,0) TO A POWER.
    KEXP= KL + ALTNAT + 0,1
    FACTRI=1,0 +(-1,0)*KEXP/2*USPIN+1,0)
C FIND THE INTEGRATED LINE INTENSITY DUE TO SPONTANEOUS EMISSION.
30  E=FACTRI*S*(NUBAR**2_AOE)**2*CINT2*EXP(-1,43879*(CINT1
    +B(VU*(KU-KU+1,0))/TROT)+2,30259*CINT3)
C SET CONSTANTS USED TO DISTRIBUTE THE ROTATIONAL LINE.
    NCENTR=1,5*(LAMCL-LAMMIN)/DELLAM
    NSTART=NCENTR-NSPRED
    IF (NSTART .LT. 1) NSTART=1
    NEND=NCENTR+NSPRED
    IF (NEND .GT. NARRAY) NEND=NARRAY
C DISTRIBUTE THE ROTATIONAL LINE.
40  DO 40 MI=NSTART,NEND
        COUNT=MI
        LAMBDA=LAMMIN+(COUNT-1,0)*DELLAM
        CSPRD3=ABS((LAMBDA-LAMCL)/WIDTHV)
        ELAM(MI)=ELAM(MI) +E*(CSPRDI*EXP(-2*TET2*CSPRD3**2)
            +CSPRD2/(1,0+4,0*CSPRDB**2) +0,016*CSPRDB*(1,0-
            2 WIDTHL/WIDTHV)*EXP(-0,4*CSPRD3**2.25)
            -0,0/3
387
    BRANCH= BRANCH + E
40  END
50  KU=KU+1,0
60  KL=KL+1,0
C HAVE BOTH BRANCHES BEEN COMPLETED.
    IF (KL .EQ. KU+1,0) GO TO 70
C WRITE P BRANCH DATA.
    WRITE(6,600) BRANCH,(FACTRI(M),M=1,5)
    BAND=BRANCH
    SYSTEM=SYSTEM+BRANCH
C SET CONSTANTS FOR THE R BRANCH.
    CSTR=0,0
    KU=KMIN
    KL=KU+1,0
    GO TO 10
C WRITE R BRANCH DATA.
70  WRITE(6,601) BRANCH,(FACTRI(M),M=1,5)
    BAND=BRANCH
    SYSTEM=SYSTEM+BRANCH
C COMPUTE APPROXIMATE BAND INTENSITY.  SEE BATES, PAGE 37.
    OR=TROT/(1,43879*B(VU))
    APPROX=CINT2*G04*(NUBAR**2*A04)**2*EXP(-1,43879*CINT1+
        2,30259*CINT3)
C WRITE ADDITIONAL DATA FOR THIS VIBRATIONAL BAND.
    WRITE(6,602) BAND,(FACTRI(M),M=1,5),APPROX,(FACTRI(M),M=1,5)
    RETURN
C FORMATS FOR WRITE STATEMENTS.
600 FORMAT(IO7X,8HP BRANCH,1X,EIO.4,5AI)
601 FORMAT(IO7X,8HP BRANCH,1X,EIO.4,5AI)
602 FORMAT(IIO5X,8HP BAND TOTAL,1X,EIO.4,5AI/
    1 91X,22HAPPROXIMATE BAND TOTAL,1X,EIO.4,5AI//)
END
SUBROUTINE ONE

COMPUTES PERPENDICULAR TRANSITIONS FOR DIATOMIC MOLECULES.

COMMON/CPLOT/LAMMIN,LAMMAX,DELLAM,NARRAY,CINT3,FACTRI(5)
COMMON/CARRAY/(LAM: 9000),(LAM: 9000)
COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
COMMON/CBAND/ALPHAU,BEU,BETAU,CAPLU,DELU,DEEU,RELU,TERM1,
               RELU,DEEU,DEEU,REEU,DEEU,REEU,DEEU,REEU,DEEU,REEU
COMMON/CTEMP/ELECT,TVIB,TROT
COMMON/CTRAN/PARTCC,NUBARO,NUBAR,NUBAR1,NUSPIN
COMMON/CWAVE/WIDTHL_WIDTHV,WIDTHRANGE
COMMON/CXTRA/INDEX,SYSTEM,TOTAL OUTPUT(12)

REAL ILAM,KU,KL,LAMBDA,LAMMAX,LAMMIN,NUBAR,NUBARO,NUSPIN
INTEGER SWITCH

C FIND THE NUMBER OF ENTRIES IN THE INTENSITY ARRAY FROM THE LINE CENTER.
C AT WHICH EACH LINE IS ASSUMED TO HAVE A CONTRIBUTION.
NSPRED=I,I+RANGE*WIDTHV/DELLAM

C SET CONSTANTS WHICH DETERMINE THE LINE SHAPE.
CSPRD2:WIDTHL/WIDTHV
CSPRD2=(1.065+0.047*CSPRD2+0.58*CSPRD2**2)*WIDTHV*1.0E-4
CSPRD3=(1.0-CAPLU)/CSPRD3
CSPRD2=CSPRD2/CSPRD3

C SET THE SIGN OF CAPLU USED IN STRENGTH EQUATIONS. APPROPRIATE TO THE
C SIGN OF DELTA LAMBDA. SEE JOHNSON, PAGE 150.
SIGN=1.0
IF (CAPLU,LT, CAPLU) SIGN=-1.0

C SET CONSTANTS FOR THE P BRANCH AND INITIALIZE THE RUNNING SUMS.
SWITCH= 1
KU=KMIN
KL=KU+1.0
BAND = 0.0
10 BRANCH=0.0

C COMPUTE AND DISTRIBUTE THE INTEGRATED INTENSITY DUE TO SPONTANEOUS
C EMISSION OF ALL SPECIFIED ROTATIONAL LINES.
DO 90 M=KMIN,KMAX

C COMPUTE THE WAVELENGTH OF THE LINE CENTER IN ANGSTROMS.
NUBAR=NUBARO +BVU*KU*(KU+1.0) -BVL*KL*(KL+1.0) -DVU*KU**2*
             (KU+1.0)**2 +OVL*KL**2*(KL+1.0)**2
LAMCL=I,OE+B/NUBAR

C IF THE LINE WAVELENGTH FALLS OUTSIDE THE SPECTRAL RANGE OF
C INTEREST, OMIT IT AND PROCEED TO THE NEXT LINE.
IF (LAMCL,LT,LAMMIN-RANGE*WIDTHV) GO TO 80
IF (LAMCL,GT,LAMMAX+RANGE*WIDTHV) GO TO 80

C FIND THE STRENGTH FACTOR.
GO TO (20,30,40)_ SWITCH

C P BRANCH STRENGTH FACTOR
20 S=(KU+1.0-SIGN*CAPLU)*(KU+2.0-SIGN*CAPLU)/(2.0*KU+1.0)
GO TO 50

C Q BRANCH STRENGTH FACTOR.
30 S=(KU+SIGN*CAPLU)**(2.0*KU+1.0)**(KU+1.0-SIGN*CAPLU)/
             2.0**KU**1.0)
GO TO 50

C R BRANCH STRENGTH FACTOR.
40 S=(KU+SIGN*CAPLU)**(KU+1.0-SIGN*CAPLU)/(2.0*KU)

C DETERMINE IF LINES ALTERNATE IN INTENSITY.
50 FACTOR=1.0
IF (ALT:AT=E,0.0) GO TO 60

C EVALUATE THE ALTERNATION FACTOR FOR HOMONUCLEAR MOLECULES. THE
C EXPONENT IN THE ALTERNATING FUNCTION IS FOUND SEPARATELY TO ENSURE
C THAT IT IS AN INTEGER BEFORE RAISING (-1.0) TO A POWER.
KEEP=KL + ALT:AT + 0.1
FACTOR=1.0 +(-1.0)**KEEP/(2.0*NUSPIN+1.0)

GO TO 10
C FIND THE INTEGRATED LINE INTENSITY DUE TO SPONTANEOUS EMISSION.

60 E=FACTOR*NUBAR*AGE*2*CINT2*EXP(-1.43879*CINT1)
   1+(9V+KU*KU+0.11/TROT+2.39259*CINT5)

C SET CONSTANTS USED TO DISTRIBUTE THE ROTATIONAL LINE.

NCENTR=I+1+LANCL/DELLAM
NSTART=NCENTR-NSPRED
IF (NSTART .LT. 1) NSTART=1
NEND=NCENTR +NSPRED
IF (NEND .GT. NARRAY) NEND=NARRAY

C DISTRIBUT THE ROTATIONAL LINE.

DO 70 M=NSTART+NEND
   COUNT=M1
   LAMBDA=LAMMIN+(COUNT-I,0)*DELLAM
   CSPRD3=ABS((LAMBDA-LAMCL)/WIDTHV}
70 ELAM(M1)=ELAM(M1) +E*(CSPRDl*EXP(-2.772*CSPRD3*_2)
   +CSPRD2/(I,0+_.O*CSPRD3**2) +0.016" CSPRD2*(I,O-
   2 WIDTHL/WIDTHV)*(EXP(-0.4*CSPRD3**2.25) -10,0/
   (10.0*CSPRD3**2.25)))

IF (NSTART .LT. 1) NSTART=1
NEND=NEND+1

C HAVE ALL THREE BRANCHES BEEN COMPLETED.

GO TO (100,110,120)_SWITCH

C OUTPUT P BRANCH INTEGRATED INTENSITY.

100 WRITE(6,600) BRANCH*(FACTRI(M) M=1,5)

C SET CONSTANTS FOR Q BRANCH.

SWITCH=2
KU=KU+1,0
KL=KL+1,0
BRANCH=BRANCH + E

10 WRITE(6,601) BRANCH*(FACTRI(M) M=1,5)

C SET CONSTANTS FOR R BRANCH.

SWITCH=3
KU=KU+1,0
KL=KL+1,0
BRANCH=BRANCH + E

120 WRITE(6,602) BRANCH*(FACTRI(M) M=1,5)

C COMPUTE APPROXIMATE BAND INTENSITY, SEE BATES, PAGE 57.

QR=TROT/(1.43879*BVU)
APPROX=CINT2*QR*(NUBAR**2*AOE)**2*EXP(-1.43879*CINT1
   1+2.39259*CINT5)

WRITE(6,603) BAND*(FACTRI(M) M=1,5)+APPROX*(FACTRI(M) M=1,5)
RETURN

C FORMATS FOR WRITE STATEMENTS.

600 FORMAT(107X,BP Branch,M1=,I4,5A1)
601 FORMAT(107X,BP Branch,M1=,I4,5A1)
602 FORMAT(107X,BR Branch,M1=,I4,5A1)
603 FORMAT(/ 105X+BAND Total,1X,IPE10,4+5A1/)

END

$ORIGIN ALPHA
$LBFTC

SUBROUTINE S2 PI2

C SUBROUTINE S2 PI2 COMPUTES DOUBLET SIGMA TO DOUBLET PI TRANSITIONS FOR DIATIC MOLECULES.

COMMON/CPLOT/LAMMIN,LAMMAX,DELLAM,NARRAY,CINT3,FACTRI(5)
COMMON/CARRAY/ILAM( 9000),ELAM( 9000)
COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
COMMON/CBAND,ALPHAU,BETAL,CApAU,CApLU,DEU,DEL,TERMU.
1 ALPHAL,BETAL,CApAL,CApLU,DEL,DEGENU,REL,TERMU
COMMON/CEXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUTII2)

SIFBTC HF0750

SUBROUTINE S2 PI2 Computes Doublet Sigma to Doublet Pi Transitions FOR Diatic Molecules.
DIMENSION NAME(16,2)
REAL LAM, JU, JU, XLAM, LAMBDA, LAMMAX, LAMMIN, NUBAR, NUBAR0,
1 NUSPIN
INTEGER SWITCH
LOGICAL FROMPI, DBLBRN
DATA (NAME(I1, M1), M2, 1, 2, M1, 1, 16)/
C PI TO SIGMA TRANS. SIGMA TO PI TRANS.
1 6H 6H R2 + 6H 6H R2
2 6H 6H R1 + 6H 6H P1
3 6H 6H R21 + 6H 6H R21
4 6H 6H OP11 + 6H 6H OP12
5 6H Q2 AND 6H OP21 + 6H Q2 AND 6H OR12
6 6HQ1 AND 6H OR12 + 6HQ1 AND 6H OR21
7 6HQ2 AND 6H OR21 + 6HP2 AND 6H PG12
8 6HR2 AND 6H PG12 + 6HR1 AND 6H RQ21
C DBLBRN IS TRUE WHEN COMPUTING TWO BRANCHES WHOSE LINES ARE ASSUMED TO
C HAVE THE SAME WAVELENGTHS.
C DBLBRN=.FALSE.
C ADJUST FACTOR USED IN INTENSITY EQUATION TO ACCOUNT FOR SPIN SPLITTING.
CINT2=CINT2/2.0
C SET CONSTANTS APPROPRIATE TO THE ELECTRONIC TRANSITION. FROMPI IS TRUE
C IF THE UPPER STATE IS DOUBLET PI.
FROMPI=.FALSE., IF (CAPLU.GT.CAPLL) FROMPI=.TRUE.
C SET COUPLING CONSTANT.
YU=CAPAU/BVU
YU=CAPAL/BVL
Y=YL
IF (FROMPI) Y=YU
C SET SWITCH, THE BRANCH IDENTIFIER, AND IPRINT, THE INDEX ON NAME WHICH
C IDENTIFIES THE BRANCH OUTPUT.
SWITCH= 0
IPRINT=0
IF (FROMPI) IPRINT=-1
C FIND THE NUMBER OF ENTRIES IN THE INTENSITY ARRAY, FROM THE LINE CENTER,
C AT WHICH EACH LINE IS ASSUMED TO HAVE A CONTRIBUTION.
NSPRED: I.I+RANGE*WIDTHV/DELLAM
C SET CONSTANTS WHICH DETERMINE THE LINE SHAPE.
CSPRD1=WIDTHL/WIDTHV
CSPRD3=(1.065+0.447*CSPRD2+0.058*CSPRD2**2)*WIDTHV*1.0E-4
CSPRD2=CSPRD2/CSPRD3
CSPRD2=CSPRD2/CSPRD3
C SET CONSTANTS FOR THE P2 BRANCH (PI TO SIGMA TRANSITION) OR
C R2 BRANCH (SIGMA TO PI TRANSITION).
BAND=0.0
K=KM1
JUM=JU-1.0
IF (FROMPI) JL=JU+1.0
C SET CONSTANTS FOR THE WAVELENGTH EQUATION.
SIGNU1=1.0
SIGNU2=1.0
C SET CONSTANTS FOR THE STRENGTH EQUATION.
SIGN1=1.0
SIGN2=1.0
CONST1=1.0
CONST2=1.0
GO TO 80
10 WRITE(6, 600) (NAME(IPRINT+M1), M1, 1, 2) BRANCH, (FACTRI(M), M=1, 16)
C SET CONSTANTS FOR THE R1 BRANCH (PI TO SIGMA TRANSITION) OR
C P1 BRANCH (SIGMA TO PI TRANSITION).
JUM=JU-0.5
JL=JU+1.0
IF (FROMPI) JL=JU+1.0
C SET CONSTANTS FOR THE WAVELENGTH EQUATION.
SIGNU1=1.0
SIGNU2=1.0
C SET CONSTANTS FOR THE STRENGTH EQUATION.
C SET CONSTANS FOR THE SR21 BRANCH (EITHER TRANSITION).
JU=K-0.5
JL=JU+1.0
C SET CONSTANTS FOR THE WAVELENGTH EQUATION.
SIGNU1=I,0
SIGNU2=-I,0
C SET CONSTANTS FOR THE STRENGTH EQUATION.
SIGNU1=-I,0
SIGNU2=-I,0
CONST1=7,0
CONST2=1,0
IF (FROMPI) CONST3=1,0
GO TO 80
30 WRITE(6,600) (NAME(IPRINT,M1),MI=I,2),BRANCH faktM,MI=M,5
C SET CONSTANTS FOR THE OP12 BRANCH (EITHER TRANSITION).
JU=K+0.5
JL=JU+1.0
C SET CONSTANTS FOR THE WAVELENGTH EQUATION.
SIGNU1=I,0
SIGNU2=1.0
C SET CONSTANTS FOR THE STRENGTH EQUATION.
SIGNU1=-I,0
SIGNU2=-I,0
CONST1=7,0
CONST2=1,0
IF (FROMPI) CONST3=1,0
GO TO 80
40 WRITE(6,600) (NAME(IPRINT,M1),MI=1,2),BRANCH faktM,MI=M,5
C SET CONSTANTS FOR THE Q2 AND QP21 BRANCHES (PI TO SIGMA TRANSITION) OR
Q2 AND QR12 BRANCHES (SIGMA TO PI TRANSITION).
DBLBRN=TRUE.
JU=K-0.5
JL=JU
C SET CONSTANTS FOR THE WAVELENGTH EQUATION.
SIGNU1=I,0
SIGNU2=1.0
C SET CONSTANTS FOR THE STRENGTH EQUATION.
SIGNU1=-I,0
SIGNU2=-I,0
SIGNU3=-I,0
SIGNU1=7,0
SIGNU2=1,0
SIGNU3=1,0
GO TO 80
50 WRITE(6,602) (NAME(IPRINT,M1),MI=1,2),BRANCH faktM,MI=M,5
C SET CONSTANTS FOR THE Q1 AND QR12 BRANCHES (PI TO SIGMA TRANSITION) OR
Q1 AND QP21 BRANCHES (SIGMA TO PI TRANSITION).
JU=K+0.5
JL=JU
C SET CONSTANTS FOR THE WAVELENGTH EQUATION.
SIGNU1=I,0
SIGNU2=1.0
C SET CONSTANTS FOR THE STRENGTH EQUATION.
SIGNU1=-I,0
SIGNU2=-I,0
SIGNU3=-I,0
SIGNU1=7,0
SIGNU2=1,0
SIGNU3=1,0
GO TO 80
60 WRITE(6,602) (NAME(IPRINT,M1),MI=1,2),BRANCH faktM,MI=M,5
C SET CONSTANTS FOR THE R2 AND RQ21 BRANCHES (PI TO SIGMA TRANSITION) OR
P2 AND PQI2 BRANCHES (SIGMA TO PI TRANSITION).
JU=K-O.5
JL=JU+1.0
IF (FROMPI) JL=JU-1.0
C SET CONSTANTS FOR THE WAVELENGTH EQUATION.
SIGNUI=I.0
SIGNU2=-I.0
C SET CONSTANTS FOR THE STRENGTH EQUATION.
SIGNS1=1.0
SIGNS2=1.0
SIGNS3=-1.0
CONSTI=-7.0
CONST2=0.0
CONST3=-7.0
GO TO 80
70 WRITE(6,6021)(NAME(IPRINT,MI),MI:I,2)DBRANCH,(FACTRI(M),M=1_5)
C SET CONSTANTS FOR THE PI AND PQI2 BRANCHES (PI TO SIGMA TRANSITION) OR
R1 AND RQ21 BRANCHES (SIGMA TO PI TRANSITION).
JU=K+0.5
JL=JU-I,0
IF (FROMRI) JL=JU+I,0
C SET CONSTANTS FOR THE WAVELENGTH EQUATION.
SIGNUI=-1.0
SIGNU2=-1.0
C SET CONSTANTS FOR THE STRENGTH EQUATION.
SIGNS1=1.0
SIGNS2=1.0
SIGNS3=-1.0
CONSTI=-7.0
CONST2=1.0
CONST3=1.0
C COMPUTE AND DISTRIBUTE THE INTEGRATED INTENSITY DUE TO SPONTANEOUS
EMISSION OF ALL SPECIFIED ROTATIONAL LINES FOR THE APPROPRIATE BRANCH.
C J IS THE ROTATIONAL QUANTUM NUMBER OF THE PI STATE. SEE REFERENCE BY
C EARLS.
80 BRANCH=0.0
J=JL
IF (FROMPI) J=JU
DO 120 M=KMIN,KMAX
C COMPUTE THE WAVELENGTH OF THE LINE CENTER IN ANGSTROMS.
NUBAR=NUBARO +BVU*((JU+0.5)**2 -CAPLU**2 +SIGNUI/2.0*SQRT(4.0*(JU+0.5)**2 -4.0*YU*CAPLU**2 +YU**2))
2 -BVL*((JL+0.5)**2 -CAPLL**2 +SIGNU2/2.0*SQRT(4.0*(JL+0.5)**2 -4.0*YL*CAPLL**2 +YL**2))
LAHCL=1.0E+8/NUBAR
C IF THE LINE WAVELENGTH FALLS OUTSIDE THE SPECTRAL RANGE OF
C INTEREST, OMIT IT AND PROCEED TO THE NEXT LINE.
IF(LAMCL,LT,LAMMIN-RANGE_WIDTHV) GO TO 110
IF(LAMCL,GT,LAMMAX+RANGE_WIDTHV) GO TO 110
C FIND STRENGTH FACTOR FOR SINGLE BRANCHES.
S=S+(2.0*J+1.0)*(4.0*J+3.0)*SIGNS2*(2.0*J+1.0)+CONST2
1 +SIGNS3*2.0*X/((16.0*(J+1.0))**2)
IF (.NOT,DBLBRN) GO TO 90
C FIND STRENGTH FACTOR FOR DOUBLE BRANCHES.
S=S+(2.0*J+1.0)**2*(14.0*J+3.0)*SIGNS1**2*(16.0*J+3.0)**2
1 *(J+1.0)**2*SIGNS1**2*(16.0*J+3.0)**2
C FIND THE INTEGRATED LINE INTENSITY DUE TO SPONTANEOUS EMISSION.
90 E=E+NUBAR**2*A0E**2*CINT2*EXP(-1.43879*CINT1)
1 +(BVU*(JU+1.0))/TROT)=2.30259*CINT3
C SET CONSTANTS USED TO DISTRIBUTE THE ROTATIONAL LINE.
NCENTR=1.5*(LAMCL-LAMMIN)/DELLAM
NSTART=NCENTR-NSPRED
IF (NSTART LT 1) NSTART=1
NEND=NCENTR+NSPRED
IF (NEND LT STNARRAY) NEND=STNARRAY
C Distribute the rotational line.

DO 100 MI = NSTART, NEND
  COUNT = MI
  LAMDA = LAMMIN + (COUNT - 1)*DELAM
  CSRD3 = ABS(LAMDA - LAMCL)/WIDTH

100 ELAM(MI) = ELAM(MI) + CSRD1*EXP(-2.772*CSRD3**2)

BRANCH = BRANCH + E
JU = JU + 1.0
JL = JL + 1.0
K = K + 1.0

C Set factors in preparation for the next branch.
  BAND = BAND + BRANCH
  SYSTEM = SYSTEM + BRANCH
  K = KMIN
  IPRINT = IPRINT + 2
  SWITCH = SWITCH + I

C Go to the appropriate branch.
  GO TO (100, 20, 30, 60, 70, 130, 1) SWITCH

C Compute approximate band intensity. See Bates, page 57.
  QR = TROT/(1.43879*BVU)
  APPROX = CINT2*QR**3*(NUBARO*2*AOE)**2*EXP(-1.43879*CINT1 +
                2.30259*CINT3)
  WRITE(6, 601) (NAME(IPRINT, MI), JU + 1, BRANCH, FACTRI(MI), MI + 1, 5),
  BAND, FACTRI(MI), MI + 1, 5, APPROX, FACTRI(MI), MI + 1, 5
  RETURN

C Formats for write statements.

FORMAT(9X, 2A6, 4HBRANCH = 4X, IPE10, 4S1)
FORMAT(9X, 2A6, 4HBRANCH = 4X, IPE10, 4S1)
FORMAT(9X, 2A6, 4HBRANCH = 4X, IPE10, 4S1)

END

*******************************************************************************

ALPHA

SUBROUTINE atomic

SUBROUTINE ATOMIC COMPUTES THE ELECTRONIC TRANSITION FOR ATOMS.

COMMON/CANNOT/LAMMIN, LAMMAX, DELAM, NARRAY, CINT3, FACTRI

COMMON/CARRAY/ILAM, ELAM(900), NARRAY(900)

COMMON/CREAD/READ1, READ2, READ3, READ4, READ5, READ6

COMMON/CBAND/ALPHAU, BETAU, ALPHAL, BETAL, CAPAL, CAPLU, DEL, DZEROL, REL, TERMU

COMMON/CBAND2/WEU, WEXU, WEXEL, WEYU, WEXE, WEXEL, WEZU, WEXZ, WEZE, DELT, TERMU

COMMON/CTEMP/TELECT, TVIB, TROT, TVIP

COMMON/CPLOT/LAMMIN, LAMMAX, DELAM, NARRAY, CINT3, FACTRI

COMMON/CREAD/READ1, READ2, READ3, READ4, READ5, READ6

COMMON/CBAND/ALPHAU, BETAU, ALPHAL, BETAL, CAPAL, CAPLU, DEL, DZEROL, REL, TERMU

COMMON/CBAND2/WEU, WEXU, WEXEL, WEYU, WEXE, WEXEL, WEZU, WEXZ, WEZE, DELT, TERMU

COMMON/CTEMP/TELECT, TVIB, TROT, TVIP

REAL ILAM, LAMMIN, LAMMAX, NAME

C Write the integrated intensity for the previously computed system.

IF (SYSTEM .NE. 0.0) WRITE(6, 600) SYSTEM, FACTRI(MI), MI + 1, 5

C Write the general heading and data for atomic transitions.

WRITE(6, 601) READ1, READ2, READ3, READ6

C Write the integrated spontaneous emission intensity for the prior atom.

*******************************************************************************

42
WRITE(6,602) NAME, SYSTEM, IFACTR(M), M=1, 5
NAME=READ6
SYSTEM=READ7
IF(TERMU.GE.0.0 .AND. DEGENU.GE.0.0) GO TO 40
READ1=WIDTHG
READ2=WIDTHL
READ3=DEGENU
READ4=TERMU
READ5=EINSTN
RETURN

40 ATOMCC=WIDTHG
TELECT=WIDTHL
Q=DEGENU
GO TO 20

C FIND THE INTENSITY FACTOR, IF NECESSARY.
50 CINT1=TERMU/TELECT
IF(IFACTR.LT.30) GO TO 90
CINT4=IFACTR
IF(CINT4.LT.CINT3) GO TO 90
IFACTR(1)=OUTPUT(12)
M=IFACTR/1000
DO 60 M1=2, 5
IFACTR(M1)=OUTPUT(M+1)
M=IFACTR/10**4*(M1)
60 C IF THIS IS NOT THE FIRST INTENSITY FACTOR, ADJUST THE ELAM ARRAY.
CINT3=Q*0.01 GO TO 80
CINT5=CINT4-CINT3
DO TO M1=NARRAY
70 ELAM(M)=ELAM(M)*EXP(2.30259*CINT5)
SYSTEM=SYSTEM*EXP(2.30259*CINT5)
TOTAL=TOTAL*EXP(2.30259*CINT5)
80 C RANGE IS THE DISTANCE FROM THE LINE CENTER, IN LINEWIDTHS, BEYOND WHICH THE
C LINE INTENSITY IS CONSIDERED ZERO.
90 IF (RANGE.GE.0.0) GO TO 95
RANGE=5.0
IF (WIDTHL.EQ.0.0) RANGE=5.0
C FIND THE VOIGT LINE WIDTH AT HALF-HEIGHT.
95 WIDTHV=WIDTHL/2.0+SQRT(WIDTHL**2/4.0+WIDTHG**2)
IF (WIDTHV.LE.0.0) GO TO 100
WIDTHV=10.0*DELLAM
WIDTH=WIDTHV
WRITE(6,701)
C FIND THE NUMBER OF ENTRIES IN THE INTENSITY ARRAY, FROM THE LINE CENTER,
C AT WHICH EACH LINE IS ASSUMED TO HAVE A CONTRIBUTION.
100 NSPRED=11+RANGE*WIDTH/DELLAM
C SET CONSTANTS WHICH DETERMINE THE LINE SHAPE.
CSPRD2=WIDTHL/WIDTHV
CSPRD3=(1.065+0.447*CSPRD2+0.058*CSPRD2**2)*WIDTHV**1.0/4
CSPRD4=(1.0+CSPRD2+CSPRD3)
CSPRD2=CSPRD2*CSPRD3
C IF THE LINE WAVELENGTH FALLS OUTSIDE THE SPECTRAL RANGE OF
C INTEREST, OMIT IT AND PROCEED TO THE NEXT LINE.
IF(LAMCL.LT.LAMMIN-RANGE*WIDTHV) GO TO 120
IF(LAMCL.GT.LAMMAX+RANGE*WIDTHV) GO TO 128
C FIND THE INTEGRATED LINE INTENSITY DUE TO SPONTANEOUS EMISSION,
E=1.580E-16*ATOMCC*DEGENU*EINSTN*EXP(-1.43879*TERMU/TELECT
+2.30259*CINT3)/(Q*LAMCL)
C SET CONSTANTS USED TO DISTRIBUTE THE ATOMIC LINE.
NCENTR=1.5+(LAMCL-LAMMIN)/DELLAM
NSTART=NCENTR-NSPRED
IF (NSTART.LE.1) NSTART=1
NEND=NCENTR+NSPRED
IF (NEND.GT.NARRAY) NEND=NARRAY
C DISTRIBUTE THE ATOMIC LINE.
DO 110 MI=NSTART,NEND
COUNT=MI
LAMBDA=LAMMIN+(COUNT-1.0)*DELLAM
CSPRD3=ABS((LAMBDA-LAMCL)/WIDTHV)
110 ELAM(MI)=ELAM(MI)+E*(CSPRD1*EXP(-2.75*CSPRD2**2)+
+CSPRD2/1.044*CSPRD3**2)*10.0+CSPRD2(1.0-
WIDTH/WIDTHV)*EXP(-0.4*CSPRD3**2)*25)+10.0/
(10.0*CSPRD3**2)*25)
SYSTEM=S YSTEM+E
TOTAL=TOTAL+E

C PRINT ATOMIC LINE INFORMATION.
  IDegen = DEGEN+ 0.1
  IRANGE = RANGE+ 0.1
WRITE(6,0603) LAMCL,IDEGEN,TERMU,EINSTN,WIDTHL,WIDTHH,WIDTHV
  LAMCL = LAMCL+ 0.1
GO TO 30

C LINE WAVELENGTH FALLS OUTSIDE SPECTRAL RANGE OF INTEREST.
120 WRITE(6,7001) LAMCL
GO TO 30

C FORMAT FOR READ STATEMENT.
500 FORMAT(6E10.4,E6.0,A6)

C FORMATS FOR WRITE STATEMENTS.
600 FORMAT(/103X,12H SYSTEM TOTAL,IX,1PE10.4,SAI)
601 FORMAT(/52X,2MATOMIC LINE SPECTRUM FOR ,A6//

C FORMATS FOR ERROR STATEMENTS.
700 FORMAT(/10X,8HLINE AT ,1PE10.4,43H ANGSTROMS FALLS OUTSIDE THE PLOT
701 FORMAT(/BX,II7HLINE WIDTHS WERE NOT INPUT FOR NEXT LINE. PROGRAM I

END

****************************************************************|

$ORIGIN ALPHA
$BFTC HFO75J

SUBROUTINE PRINT(NEWCAS)
C SUBROUTINE PRINT TABULATES SPECTRAL INTENSITY VS WAVELENGTH ON THE
C WRITTEN OUTPUT.
C IN THIS SUBROUTINE, THE ILAM ARRAY, WHICH NOW CONTAINS WAVELENGTHS, WILL
C BE NAMED LAMBDA.

COMON/CPLOT/LAMMAX,LAMMIN,LAMMAX(900),ELAM(900)
COMMON/CARRAY/LAMBDA(9000),ELAM(9000)
COMMON/CREAD/READ1,READ2,READ3,READ4,READ5
COMMON/CRAND/ALPHAU,BEU,BETAL,CAPAU,CAPLL,DEL,DZEROU
COMMON/CBAND2/WEU,WEXEU,WEYEU,WEZEU,BVL,DVL_ NUSPIN
COMMON/CTEMP/TELECT,TVIB,TROT
COMMON/CWIDTH/WIDTHL_WIDTHV,RANGE
COMMON/CTRAN/PARTCC,NUBARO,0.0,EINTN,CINT2,KMIN,KMAX
COMMON/CXTRA/NFILE,SYSTEM,TOTAL,OUTPUT(12)
REAL LAMBDA,LAMMAX,LAMMIN

LOGICAL NEWCAS
DATA LOG/6HLOG
C WRITE GENERAL HEADING AND READ A CARD SPECIFYING WHETHER THE
C INTENSITIES ARE TO BE PRINTED AS LINEAR OR LOG VALUES.
WRITE(6,600)
   IF(NEWCAS) GO TO 50
   READ (5,500) KIND
   IF(KIND .NE. LOG) GO TO 50
   C A LOG OUTPUT IS DESIRED.
   C WRITE HEADING FOR THE LOG OUTPUT, ENSURE THAT THE LOG OF ZERO WILL
   C NOT BE TAKEN, AND APPLY THE INTENSITY FACTOR.
   WRITE(6,601)
      DO 10 M=1,NARRAY
      IF (ELAM(M) .EQ. 0.0) ELAM(M):=1.0E-38
      ELAM(M)+ALOG10(ELAM(M)) - CINT3

44
NWRITE=NARRAY/4
N1=NWRITE+1
N2=2*NWRITE+1
N3=3*NWRITE+1

C PRINT THE LAMBDA VERSUS LOG(ELAM) VALUES IN FOUR COLUMNS ACROSS THE PAGE.
DO 20 M=1,NWRITE
   WRITE(6+602) LAMBDA(M),ELAM(M)
   1 N1=N1+1
   N2=N2+1
   N3=N3+1
20

C IS THE PRINTING COMPLETED. IF SO, RETURN TO THE MAIN PROGRAM.
IF (4*NWRITE.EQ.NARRAY) RETURN
NWRITE=NARRAY-4*NWRITE

C WRITE THE REMAINING VALUES AND RETURN TO THE MAIN PROGRAM.
DO 30 M=1,NWRITE
   WRITE(6+603) LAMBDA(N1),ELAM(N1)
   30 N1=N1+1
C IS THE PRINTING COMPLETED. IF SO, RETURN TO THE MAIN PROGRAM.
IF (4*NWRITE.EQ.NARRAY) RETURN

C A LINEAR OUTPUT IS DESIRED.
C WRITE THE HEADING FOR THE LINEAR OUTPUT.
50 WRITE(6+605)
NWRITE=NARRAY/4
N1=NWRITE+1
N2=2*NWRITE+1
N3=3*NWRITE+1
C PRINT THE LAMBDA VERSUS ELAM VALUES IN FOUR COLUMNS ACROSS THE PAGE.
DO 60 M=1,NWRITE
   WRITE(6+606) LAMBDA(M),ELAM(M),(FACTRI(M),MI=1,5),MI=1,5
   1 N1=N1+1
   N2=N2+1
   N3=N3+1
60

C IS THE PRINTING COMPLETED. IF SO, RETURN TO THE MAIN PROGRAM.
IF (4*NWRITE.EQ.NARRAY) RETURN
NWRITE=NARRAY-4*NWRITE

C WRITE THE REMAINING VALUES AND RETURN TO THE MAIN PROGRAM.
DO 70 M=1,NWRITE
   WRITE(6+607) LAMBDA(N1),ELAM(N1),(FACTRI(M),MI=1,5)
   70 N1=N1+1
C A LINEAR OUTPUT IS DESIRED.
C WRITE THE HEADING FOR THE LINEAR OUTPUT.
50 WRITE(6+605)
NWRITE=NARRAY/4
N1=NWRITE+1
N2=2*NWRITE+1
N3=3*NWRITE+1
C PRINT THE LAMBDA VERSUS ELAM VALUES IN FOUR COLUMNS ACROSS THE PAGE.
DO 60 M=1,NWRITE
   WRITE(6+606) LAMBDA(M),ELAM(M),(FACTRI(M),MI=1,5),MI=1,5
   1 N1=N1+1
   N2=N2+1
   N3=N3+1
60

C IS THE PRINTING COMPLETED. IF SO, RETURN TO THE MAIN PROGRAM.
IF (4*NWRITE.EQ.NARRAY) RETURN
NWRITE=NARRAY-4*NWRITE

C WRITE THE REMAINING VALUES AND RETURN TO THE MAIN PROGRAM.
DO 70 M=1,NWRITE
   WRITE(6+607) LAMBDA(N1),ELAM(N1),(FACTRI(M),MI=1,5)
   70 N1=N1+1

C FORMAT FOR READ STATEMENT.
500 FORMAT(66X,A6)
C FORMATS FOR WRITE STATEMENTS.
600 FORMAT(//49X,29HTABULATION OF COMPUTED SPECTRUM//)
601 FORMAT(1X,13X,WAVELENGTH LOG 10(INTENSITY),X)
   1 4(3X,29HANGSTROMS W/CM2-MICRON-SR),X)
602 FORMAT(I4(3X,29HANGSTROMS W/CM2-MICRON-SR),X)
603 FORMAT(I4(3X,29HANGSTROMS W/CM2-MICRON-SR),X)
604 FORMAT(I4(3X,29HANGSTROMS W/CM2-MICRON-SR),X)
605 FORMAT(I4(3X,21HINTENSITY,8X)
   1 4(3X,27HANGSTROMS W/CM2-MICRON-SR,2X)//)
606 FORMAT(I4(3X,27HANGSTROMS W/CM2-MICRON-SR,2X)//)
607 FORMAT(I4(3X,27HANGSTROMS W/CM2-MICRON-SR,2X)//)

END
COMMON/CTEMP/TELECT,TVIB,TROT
COMMON/CTRAIN/PARNCC,NUMR=Q,AOE,CINT1,CINT2,KMIN,KMAX
COMMON/CEXTRA/INDEX,INFILE,SYSTEM,TOTAL,OUTPUT

REAL LAM2,LAMMAX,LAMMIN,LAMDA,

C WRITE GENERAL HEADING AND READ WAVELENGTH LIMITS FOR INTEGRATION
C INTERVAL.
   WRITE(6,600)
   READ(5,500) LAM1, LAM2
C INITIALIZE INTEGRATED INTENSITY FOR THIS INTERVAL.
   TOTALI=0.0
C IF THE UPPER WAVELENGTH LIMIT WAS INPUT FIRST, WRITE AN ERROR
C MESSAGE AND OMIT THIS INTERVAL.
   IF (LAM2 .LE. LAM1) GO TO 70
C IF WAVELENGTH LIMITS ARE OUTSIDE SPECTRAL RANGE CONSIDERED, SET
C INTEGRATION LIMITS TO APPROPRIATE END WAVELENGTH.
   IF (LAM1 .LT. LAMMIN) LAMI=LAMMIN
   IF (LAM2 .GT. LAMMAX) LAM2=LAMMAX
C FIND INDICES IN INTENSITY ARRAY TO BE INCLUDED IN INTEGRATION.
   NSTART= 1.0 +LAM2-LAMMIN)/DELLAM
   NEND= 1.0 +LAM2-LAMMIN)/DELLAM
C TEST INTERVAL LIMITS.
   IF (NSTART .LT. NEND) GO TO 20
C THE INTERVAL IS BOUNDED BY CONSECUTIVE ENTRIES IN THE LAMBDA ARRAY.
   SLOPE=(ELAM(NSTART+1)-ELAM(NSTART))/DELLAM
   TOTALI=(SLOPE*(LAM1-LAMMIN)+ELAM(NSTART))+(SLOPE*(LAM2-LAMMIN)+ELAM(NSTART))*
   (LAM2-LAMI)/2.0E+4
   GO TO 50
C IS THERE A RIGHT-HAND INCREMENT.
   IF (NEND.EQ.NARRAY) GO TO 30
C COMPUTE INTEGRATED INTENSITY FROM RIGHT-HAND INCREMENTAL AREA.
   ELAMI=(ELAM(NEND+1)-ELAM(NEND))*LAM2-LAMMIN)/DELLAM
   TOTALI=TOTALI+ELAMI+ELAM(NENDI)
   GO TO 50
C COMPUTE INTEGRATED INTENSITY FROM LEFT-HAND INCREMENTAL AREA.
   ELAMI=(ELAM(NSTART)-ELAM(NSTART+1))*(LAM2-LAMI)/DELLAM
   TOTALI=TOTALI+ELAMI+ELAM(NSTART+I)
   GO TO 50
C DO INTERVAL LIMITS BOUND A SINGLE ENTRY IN THE LAMBDA ARRAY.
   IF (NEND .EQ. NSTART+I) GO TO 50
C COMPUTE INTEGRATED INTENSITY FROM CENTRAL INCREMENTAL AREAS.
   NSTART=NSTART+2
   DO 40 M=NSTART,NEND
   TOTALI=TOTALI+(ELAM(M)+ELAM(M-I))*DELLAM/2.0E+4
   GO TO 40
C WRITE WAVELENGTH LIMITS AND RESULTING VALUE OF INTEGRATION.
   WRITE(6,601) LAMI,LAM2,TOTALI.(FACTRI(M),M:lt5)
C IF INTEGRATION HAS BEEN
C COMPLETED FOR ALL SPECIFIED INTERVALS,
C RETURN TO MAIN PROGRAM.
   IF (NINTRV.NE.O) GO TO 10
   RETURN
C THERE IS AN ERROR IN THE LIMITS FOR THE INTEGRATION INTERVAL.
   WRITE(6,605) LAM1,LAM2
   GO TO 60

FORMAT(2ElO.O)
C FORMATS FOR WRITE STATEMENTS.
600 FORMAT(///50X,31HINTEGRATED SPECTRAL INTENSITIES//
   i 35X,HLOWER WAVELENGTH 10X,HUPPER WAVELENGTH 10X,HINTEGRATED//
   i 35X,5HINIT1X,5HINIT2X,5HINTENSITY//
   3 35X,9HANGSTROMS17X,9HANGSTROMS'ITX'BHW/CM2-SR//)
601 FORMAT(35X,1PE10,4,16X,E10,4,16X,E10,4,5A1)
C FORMAT FOR ERROR STATEMENT.

700 FORMAT(3X,'THE LOWER LIMIT ',L11.4,' IS GREATER THAN THE UPPER LIMIT ',L11.4,' AND INTEGRATION WAS NOT PERFORMED.')
END

$ORIGIN ALPHA
$IBMORT HFO75L

SUBROUTINE SLIT(NSLIT)
C SUBROUTINE SLIT COMPUTES THE OUTPUT SIGNAL GIVEN BY A SPECIFIED INSTRUMENT SENSITIVITY.
C IN THIS SUBROUTINE, THE LAM ARRAY, WHICH NOW CONTAINS WAVELENGTHS, WILL BE NAMED LAMBDA.
COMMON/COLUMN/LAMMIN,LAMMAX,DELAM,N.ARRAY,CINT3,FACCTR1(5)
COMMON/CARRAY/LAMIN,9000,LAMIN,9000)
COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
COMMON/CBAND/LAMIN,BET,A,DELAM,DELAM,REU,TERMU,
1. ALPHABETALCAP,ALPHACAP,DELAM,DELAM,REU,TERMU,
COMMON/CBAND2/WEU,WEU,WEU,WEU,WEU,BVU,DVU,DEGENU,MO,ALTRAT,
1. WEU,WEU,WEU,WEU,WEU,BVU,DVU,NUSPI
COMMON/CTEMP/TELECT,TVI8,TROT
COMMON/CWIDTH/WIDTHL,WIDTHV,RANGE
COMMON/CXTRA/INDEX,AFILE,SYS,TOTAL,OUTPUT(12)
COMMON/CTRAN/PARTCC,NBARO,QA,OE,CINT1,CINTZ,KMIN,KMAX
COMMON/CEXTRA/INDEX,NFILE,SYSTEM,TOTAL,OUTPUT(12)
DIMENSION LAM(IOO),RSLIT(IOO),LAMR(IOO),LAMS(IOO),LSAV(IOO)
REAL LAMI,LAM2,LAM,LAMBDA,LAM,LAM,LAM,LAM,LAM,LAM,LAM,LAM,LAM,LAM,LAM,REU
INTEGER BLOCK_FACTR1,SCAN,FLAG
DATA SLIT1/3HSLIT/

C WRITE THE GENERAL HEADING AND INITIALIZE THE COUNTER SPECIFYING HOW MANY SLIT CASES HAVE BEEN COMPLETED.
WRITE(6,600)
MSLIT=0

C ARE ALL THE DESIRED SLIT CASES COMPLETED? IF SO, RETURN TO THE MAIN PROGRAM.
5 IF(MSLIT.EQ.NSLIT) RETURN

C THIS IS THE STARTING POINT FOR THE CONSIDERATION OF EACH NEW SLIT CASE.

6 READ(5,50O) SEARCH
IF(SEARCH.NE.SLIT1) GO TO 6

C INITIALIZE THE INSTRUMENT OUTPUT SIGNAL.
SIGNAL=0.0
WRITE(6,616)

C WAS THE UPPER SCAN LIMIT INPUT LESS THAN OR EQUAL TO THE LOWER LIMIT.
C IF SO, WRITE AN ERROR MESSAGE AND OMIT THIS SLIT.
IF(SCAN.EQ.1.AND.LAM2.LE.LAMI) GO TO 272

C IS THE SLIT FUNCTION SPECIFIED BY A GAUSSIAN CURVE OR BY A SET OF LINEAR SEGMENTS.
        IF(NPOINT.EQ.0) GO TO 25

C THE SLIT FUNCTION IS SPECIFIED BY LINEAR SEGMENTS. READ IN.
READ(5,GOO) (LAM(M),RSLIT(M),M=I,NPOINT)
WRITE(6,6O3)
WRITE(6,6O4) (LAM(M),RSLIT(M),M=I,NPOINT)

C WRITE HEADINGS FOR THE APPROPRIATE CASE.
        IF(SCAN.NE.1) WRITE(6,601) MSLIT
        IF(SCAN.EQ.1) WRITE(6,602) MSLIT,LAMI,LAM2,STEP

C IF AN ERROR WAS DETECTED IN THE PRIOR CASE, READ THROUGH THE REMAINING CARDS.
6 READ(5,SOO) SEARCH
IF(SERACH.NE.NE.SLIT1) GO TO 6

C WRITE THE CARD THAT SPECIFIES THE TYPE OF INSTRUMENT SENSITIVITY TO BE CONSIDERED.
C NUMERO: NUMBER OF ARRAY ELEMENTS SPECIFYING SLIT FUNCTION. IF
C NPOINT=0, THE SLIT FUNCTION IS SPECIFIED BY A GAUSSIAN CURVE.
4 SCAN= 1 SPECIFIES A SCANNING SLIT CASE. SCAN=0 SPECIFIES A FIXED
C SLIT CASE.
C STEP= DISTANCE IN ANGSTROMS THAT THE SLIT IS MOVED FOR EACH STEP OF
C THE SCAN.
C LAMS1= STARTING WAVELENGTH OF THE SCAN FOR A SCANNING SLIT. LOCATION
C OF THE SLIT CENTER LINE FOR A FIXED LINEAR SLIT.
C LAM2= STOPPING WAVELENGTH OF THE SCAN FOR A SCANNING SLIT.
C NRLAMS= NUMBER OF ARRAY ELEMENTS IN THE SPECTRAL CALIBRATION ARRAY.
READ(5,SOO) NPOINT,SCAN,STEP,LAMSL,SLAM2,NRLAMS

C WRITE HEADING FOR THE APPROPRIATE CASE.
        IF(SCAN.NE.1) WRITE(6,601) MSLIT
        IF(SCAN.NE.1) WRITE(6,602) MSLIT,LAMI,LAM2,STEP

C WAS THE UPPER SCAN LIMIT INPUT LESS THAN OR EQUAL TO THE LOWER LIMIT.
C IF SO, WRITE AN ERROR MESSAGE AND OMIT THIS SLIT.
        IF(SCAN.NE.1.AND.LAM2.LE.LAMI) GO TO 272

C IS THE SLIT FUNCTION SPECIFIED BY A GAUSSIAN CURVE OR BY A SET
C OF LINEAR SEGMENTS.
        IF(NPOINT.EQ.0) GO TO 25

C THE SLIT FUNCTION IS SPECIFIED BY LINEAR SEGMENTS. READ IN.
        IF(SCAN.NE.1) WRITE(6,603) (LAM(M),RSLIT(M),M=I,NPOINT)
        IF(SCAN.NE.1) WRITE(6,6O4) (LAM(M),RSLIT(M),M=I,NPOINT)
C DO THE WAVELENGTHS SPECIFYING THE SLIT FUNCTION INCREASE MONOTONICALLY. IF NOT, WRITE AN ERROR MESSAGE AND Omit THIS SLIT.
   M=NP0INT-1
   DO 10 M=1,M+1
      IF(LAM(M) .GE. LAM(M+1)) GO TO 265
   CONTINUE
C FIND THE PEAK OF THE SLIT FUNCTION AND COMPUTE THE EFFECTIVE WIDTH OF THE
C SLIT FUNCTION SPECIFIED BY LINEAR SEGMENTS.
   WIDTH=0.0
   RMAX=0.0
   DO 15 M=1,NPOINT
      IF(RSLIT(M) .GT. RMAX) RMAX=RSLIT(M)
      M=NP0INT-1
   DO 20 M=1,M+1
      WIDTH=WIDTH+0.5*(RSLIT(M)+RSLIT(M+1))*(LAM(M+1)-LAM(M))/RMAX
   CONTINUE
C READ THE DATA DENOTING THE CENTER OF THE SLIT FUNCTION AND THE CALIBRATION
C FACTOR USED TO SPECIFY THE INSTRUMENT SENSITIVITY IF THIS IS A FIXED
C WAVELENGTH RADIOMETER.
   READ(5,503) LAMCL, RLMCL
C IS THE SPECIFIED CENTER OF THE SLIT FUNCTION COMPATIBLE WITH THE SLIT
C FUNCTION DATA. IF NOT, WRITE AN ERROR MESSAGE AND OMIT THIS SLIT.
   IF(LAMCL .LT. LAM(1) .OR. LAMCL .GT. LAM(NPOINT)) GO TO 266
   GO TO 30
C THE SLIT FUNCTION IS SPECIFIED BY A GAUSSIAN FUNCTION. PRINT THE
C HEADING AND READ THE DEFINING DATA.
   WRITE(6,607)
   READ(5,501) LAMCL, RLMCL, WIDTH
C IS THIS A SPECTROGRAPH OR SCANNING SPECTROMETER CASE.
   IF(SCAN.EQ.1) GO TO 45
C THIS IS A FIXED WAVELENGTH RADIOMETER.
   IF(NPOINT .EQ. 0) GO TO 40
C PRINT ADDITIONAL LINEAR SLIT DATA.
   WRITE(6,605) LAMCL, LAMSI, RLMCL, WIDTH
C POSITION THE SLIT AT THE SPECIFIED WAVELENGTH.
   SHIFT=LAMSI-LAMCL
   DO 35 M=1,NPOINT
      LAM(M)=LAM(M)+SHIFT
   CONTINUE
C IF PART OR ALL OF THE INSTRUMENT SENSITIVITY LIES OUTSIDE THE
C COMPUTED SPECTRUM, WRITE AN ERROR MESSAGE AND OMIT THIS SLIT.
   IF(LAM(1) .LT. LAMDA(1)) GO TO 260
   IF(LAM(NPOINT) .GT. LAMDA(NARRAY)) GO TO 260
   GO TO 125
C PRINT THE GAUSSIAN INPUT DATA.
   WRITE(6,608) LAMCL, RLMCL, WIDTH
   TEST1=LAMDA(1)-(LAMCL-3.0*WIDTH)
   IF(TEST1 .GE. 0.0) GO TO 65
   LAMSI=LAMSI+TEST1
   DO 60 M=1,NPOINT
      TEST2=LAMDA(NARRAY)-(LAMCL+3.0*WIDTH)
      IF(TEST2 .LE. 0.0) GO TO 155
      GO TO 60
   CONTINUE
C THIS IS A SPECTROGRAPH OR A SCANNING SPECTROMETER CASE. POSITION THE
C SLIT AT THE START OF THE SCAN AND TEST THE SPECIFIED END POINTS OF
C THE DESIRED SPECTRAL COVERAGE.
   IF(NPOINT .EQ. 0) GO TO 70
C THE SLIT FUNCTION IS SPECIFIED BY A LINEAR SLIT.
C PRINT ADDITIONAL SLIT DATA.
   WRITE(6,606)
   WRITE(6,604) LAMCL, WIDTH
C POSITION THE LINEAR SLIT AT THE SPECIFIED STARTING WAVELENGTH FOR THE SCAN.
   SHIFT=LAMSI-LAMCL
   DO 55 M=1,NPOINT
      LAM(M)=LAM(M)+SHIFT
   CONTINUE
C TEST THE INPUT DATA FOR THE LINEAR SCANNING SLIT.
C IF PART OR ALL OF THE INSTRUMENT SENSITIVITY WILL FALL OUTSIDE THE
C COMPUTED SPECTRUM, MAKE THE APPROPRIATE ADJUSTMENT AND WRITE A MESSAGE
C INDICATING THIS WAS DONE.
   TEST3=LAMDA(1)-LAM(1)
   IF(TEST3 .LE. 0.0) GO TO 65
   LAMSI=LAMSI+TEST3
   GO TO 60
C 48
C PRINT THE GAUSSIAN SLIT DATA.
70 WRITE(6,609) WIDTH
C TEST THE INPUT DATA FOR THE GAUSSIAN SCANNING SLIT.
C IF PART OR ALL OF THE INSTRUMENT SENSITIVITY WILL FALL OUTSIDE THE
C COMPUTED SPECTRUM, MAKE THE APPROPRIATE ADJUSTMENT AND WRITE A MESSAGE
C INDICATING THIS WAS DONE.
75 IF(TEST1.LE.O.O) GO TO 77
TEST2=LAMBDA(NARRAY)-(LAMS2+3.0*WIDTH)
77 IF(TEST2.LT.O.O) LAMS2=LAMS2+TEST2
IF(TEST1.GT.O.O.OR,TEST2.LT.O.O) WRITE(6,702) LAMSI,LAMS2,STEP
C POSITION THE SLIT AT THE SPECIFIED STARTING WAVELENGTH OF THE SCAN.
LAMC=LAMSI
C READ AND PRINT DATA SPECIFYING SPECTRAL CALIBRATION OF SCANNING SLIT.
READ(5,5021)(LAMR(M),RLAM(M),M=I,NRLAMS)
WRITE(6,604)(LAMR(M), RLAM(M),M=I_NRLAMS)
C IF THE WAVELENGTH VALUES OF THE SPECTRAL CALIBRATION DO NOT INCREASE
C MONOTONICALLY, WRITE AN ERROR MESSAGE AND OMIT THIS SLIT.
90 CONTINUE
C IF THE END POINTS OF THE SPECTRAL CALIBRATION DO NOT BOUND THE
C SCANNING RANGE, WRITE AN ERROR MESSAGE AND OMIT THIS SLIT.
95 IF(LAMSI.LT.LAMR(1)) GO TO 115
IF(LAMSI.GT.LAMR(NRLAMS)) GO TO 115
C SET THE INITIAL VALUES OF COUNTERS AND WAVELENGTHS FOR THE SCAN.
NSIGL=1
LAMS1=LAMSI
BLOCK=1
FLAG=0
NSF=0
C THIS IS THE STARTING POINT FOR EACH STEP OF THE SCAN.
C LOCATE THE SLIT CENTER WAVELENGTH BETWEEN THE PROPER ELEMENTS IN
C THE SPECTRAL CALIBRATION ARRAY.
105 IF((LAMCL.GE.LAMR(NRLAM))AND,(LAMCL.LE.LAMR(1))) GO TO 270
115 NRLAM= NRLAM+1
120 CONTINUE
C FIND THE SPECTRAL CALIBRATION RLAMCL AT THE SLIT CENTER FOR THIS
C STEP OF THE SCAN.
125 NSTART=1+1+(LAM(1)-LAMBDA(1))/DELLAM
N1=NSTART
N2=N1+1
M1=1
M2=2
C COMPUTE THE SPECTRAL INTENSITY AT THE LEFT-HAND END POINT OF
C THE SLIT FUNCTION.
LAMI=LAM(1)
RSLITI=RSLIT(1)
ELAMI=ELAM(N1)+1+(LAM(n21-LAM(1))*(ELAM(N1)+ELAM(N2))
/1 DELLLAM
C IS THE RIGHT-HAND POINT OF THE INTERVAL IN THE SPECTRUM OR SLIT
C FUNCTION ARRAY.
135 IF(LAMBDA(N2)+LT+LAM(N2)) GO TO 140
C THE RIGHT-HAND POINT OF THE INTERVAL IS IN THE SLIT FUNCTION ARRAY.

LAM2=LAM(N2)
RSLIT2=RSLIT(N2)
ELAM2=ELAM(N2)+(LAMBDA(N2)-LAM(N2))*RSLIT(N2)
N1=M1+1
N2=M2+1
GO TO 145

C THE RIGHT-HAND POINT OF THE INTERVAL IS IN THE SPECTRUM ARRAY.

140 LAM2=LAMDA(N2)
RSLIT2=RSLIT(N2)+(LAM(N2)-LAMDA(N2))*RSLIT(N1)-RSLIT(N2))
/ (LAM(N2)-LAM(N1)}
ELAM2=ELAM(N2)
N1=M1+1
N2=N2+1

C GENERATE THE LINEAR SLIT INSTRUMENT OUTPUT SIGNAL.

145 SIGNAL=SIGNAL *(ELAMIRSLIT1*ELAM2*RSLIT2)*RLAMCL*
/ (LAM2-LAM1)/2.0E+4

C IS THE INTEGRATION FOR THIS SLIT OR THIS STEP IN THE SCAN COMPLETE.

IF(LAM(NPOINT)-LAM2.LE.0.1*DELLAM) GO TO 150

C MOVE TO THE NEXT INTERVAL.

C THE LEFT-HAND POINT OF THE NEW INTERVAL IS THE RIGHT-HAND POINT OF
C THE PRIOR INTERVAL.

LAM1=LAM2
RSLIT1=RSLIT2
ELAM1=ELAM2
GO TO 135

C DIVIDE BY THE SLIT WIDTH TO YIELD THE INSTRUMENT OUTPUT
C AT THIS WAVELENGTH.

150 SIGNAL=SIGNAL/WIDTH/1.0E-04
GO TO 165

C THE INSTRUMENT SENSITIVITY IS SPECIFIED BY A GAUSSIAN CURVE.
C THE INTEGRATION SCHEME FOR GAUSSIAN SLITS BEGINS HERE.
C FIND INDICES IN THE SPECTRUM ARRAY TO BE INCLUDED IN THE INTEGRATION.

155 NSTART=1.1+(LAMCL-3.0*WIDTH-LAM(N1))/DELLAM
NEND=6.0*WIDTH/DELLAM+NSTART

C SET THE INITIAL INDEX VALUES FOR THE INTEGRATION.

N1=NSTART
N2=N1+1

C COMPUTE THE PRODUCT OF SPECTRAL INTENSITY AND INSTRUMENT SENSITIVITY
C AT THE LEFT-HAND SIDE OF THE INTEGRATION ELEMENT.

ELAM1=ELAM(N1)*RLAMCL*EXP(-2.772*(LAM(N1)-LAMCL)/WIDTH)**2

C COMPUTE THE PRODUCT OF SPECTRAL INTENSITY AND INSTRUMENT SENSITIVITY AT
C THE RIGHT-HAND SIDE OF THE INTEGRATION ELEMENT.

160 ELAM2=ELAM(N2)*RLAMCL*EXP(-2.772*(LAM(N2)-LAMCL)/WIDTH)**2

C GENERATE THE GAUSSIAN SLIT INSTRUMENT OUTPUT SIGNAL.

SIGNAL=SIGNAL+(ELAM1*ELAM2*DELLAM/2.0E+4
N1=N1+1
N2=N2+1

C IS THE INTEGRATION FOR THIS SLIT OR THIS STEP IN THE SCAN COMPLETE.

IF(N2.GT. NEND) GO TO 161
ELAM=ELAM2
GO TO 165

C DIVIDE BY THE APPROPRIATE SLIT WIDTH TO YIELD THE INSTRUMENT OUTPUT
C AT THIS WAVELENGTH.

161 SIGNAL=SIGNAL/(WIDTH/1.0E39C-04)

C IS THIS A SCANNING SLIT CASE.

165 IF(SCAN .NE. 1) GO TO 255

C THIS IS A SCANNING SLIT CASE.

C IS THE SCAN COMPLETED.

C IF(FLAG.EQ.1) GO TO 250

C IS A DATA BLOCK CONTAINING 500 ENTRIES FROM THIS SCAN COMPLETED, IF SO, GO
C TO THE PORTION OF THE SUBROUTINE WHERE THE DATA BLOCK WILL BE PRINTED ON
C THE OUTPUT SHEET.

IF(NSIGLN.EQ.500) GO TO 250
C IS THE NEXT STEP THE LAST FOR THIS SCAN.

180 TEST=LAMS2-LAMNSIGLM
IF(TEST.LT.EQ.STEP) GO TO 200

C SET THE COUNTERS AND WAVELENGTHS FOR THE NEXT STEP OF THE SCAN.

NSTEP=NSTEP+1
COUNT=NSTEP
LAMCL=LAMSI+COUNT*STEP

C IF A DATA BLOCK WAS JUST PRINTED (NSIGLM=500), READJUST THE COUNTER NSIGLM.

IF(NSIGLM.LT.500) GO TO 185
NSIGLM=1
LAMS(1)=LAMSI+COUNT*STEP
GO TO 190

185 NSIGLM=NSIGLM+1
LAMS(NSIGLM)=LAMSI+COUNT*STEP

190 IF(NPOINT.EQ.0) GO TO 225

C SAVE THE WAVELENGTHS OF THE SLIT FUNCTION AT THE FIRST SCANNING LOCATION.

IF(NSTEP.GT.1) GO TO 196
DO 195 M=1,NPOINT
195 LAMSAV(M)=LAM(M)
196 DO 197 M=1,NPOINT
197 LAM(M)=LAMSAV(M)+COUNT*STEP
GO TO 223

C SET UP THE LAST STEP OF THE SCAN.

200 FLAG=1
LAMCL=LAMS2
C IF A DATA BLOCK WAS JUST PRINTED, READJUST THE COUNTER NSIGLM.

IF(NSIGLM.LT.500) GO TO 205
NSIGLM=1
LAMS(1)=LAMS2
GO TO 210

205 NSIGLM=NSIGLM+1
LAMS(NSIGLM)=LAMS2

210 IF(NPOINT.EQ.0) GO TO 225
DO 215 M=1,NPOINT
215 LAM(M)=LAM(M)+TEST
C RE-INITIALIZE SIGNAL FOR THE NEXT STEP OF THE SCAN.

225 SIGNAL=0.0
GO TO 95

C IF THIS IS THE FIRST DATA BLOCK, PRINT THE SCAN DATA HEADING ON THE
C OUTPUT SHEET.

250 IF(BLOCK.EQ.1) WRITE(6,612)

C PRINT THE SCAN DATA ON THE OUTPUT SHEET.

WRITE(6,613) (LAMS(M),SIGLAM(M),FACTRI(M1)(MI=I'5'),M=I,NSIGLM)

C IS THIS SCAN CASE COMPLETED.

IF(FLAG .GT.4) GO TO 5

C THE SCAN CASE IS NOT COMPLETED. CONTINUE THE SCAN.

BLOCK=BLOCK+1
GO TO 180

C WRITE THE FIXED WAVELENGTH RADIOMETER DATA ON THE OUTPUT SHEET.

255 WRITE(6,615) SIGNAL,(FACTRI(M1)(MI=1'5'),M=1,NSIGLM)
GO TO 95

C THERE IS AN ERROR IN THE SLIT INPUT DATA. WRITE AN ERROR MESSAGE
C AND CONTINUE.

C ALL OR PART OF THE FIXED SLIT LIES OUTSIDE THE COMPUTED SPECTRUM.

C WAVELENGTHS SPECIFYING THE LINEAR SLIT FUNCTION DO NOT INCREASE
C MONOTONICALLY.

C SPECIFIED CENTER OF THE SLIT FUNCTION LIES OUTSIDE THE SPECIFIED SLIT
C FUNCTION.
WRITE(6,606)
WRITE(6,500) LAMCL,WIDTH
WRITE(6,704)
GO TO 5

C WAVELENGTHS OF SPECTRAL CALIBRATION DO NOT INCREASE MONOTONICALLY.

WRITE(6,701)
GO TO 5

C WAVELENGTHS SPECIFYING THE SPECTRAL CALIBRATION
C DO NOT BOUND THE DESIRED SCAN RANGE.

WRITE(6,703)
GO TO 5

C UPPER SCAN LIMIT WAS INPUT LESS THAN OR EQUAL TO THE LOWER LIMIT.

WRITE(6,705)
GO TO 5

C FORMATS FOR READ STATEMENTS.

500 FORMAT(I5_4X,I19_4X,3ElO.O,7X)  
501 FORMAT(3E10.O)  
502 FORMAT(6E10.O)  
503 FORMAT(2E10.O)  
504 FORMAT(2E13.O)  
505 FORMAT(1A4)  

C FORMATS FOR WRITE STATEMENTS.

600 FORMAT(///,1 34X_63HDETECTOR OUTPUT SIGNAL GIVEN BY A SPECIFIED INSTRUMENT RESPONSE///)  
601 FORMAT(3E10.O)  
602 FORMAT(6E10.O)  
603 FORMAT(2E10.O)  
604 FORMAT(2E13.O)  
605 FORMAT(1A4)  

C FORMATS FOR WRITE STATEMENTS.

606 FORMAT(///,1 34X_63HDETECTOR OUTPUT SIGNAL GIVEN BY A SPECIFIED INSTRUMENT RESPONSE///)  
607 FORMAT(3E10.O)  
608 FORMAT(6E10.O)  
609 FORMAT(2E10.O)  
610 FORMAT(2E13.O)  
611 FORMAT(1A4)  

C FORMATS FOR ERROR STATEMENTS.

700 FORMAT(///,1 34X_63HDETECTOR OMITTED BECAUSE PART OR ALL OF SENSITIVITY LIES OUTSIDE COMPUTED SPECTRUM///)  
701 FORMAT(///,1 34X_63HDETECTOR OMITTED BECAUSE WAVELENGTHS DO NOT INCREASE MONOTONICALLY///)  
702 FORMAT(///,1 34X_63HINPUT DATA FOR LAM1 OR LAM2 WOULD HAVE ALLOWED PORTION OR ALL OF THE INSTRUMENT SENSITIVITY TO LIE OUTSIDE THE SPECTRAL RANGE SPECIFIED///)  
703 FORMAT(///,1 34X_63HINPUT DATA FOR LAM1 OR LAM2 WOULD HAVE ALLOWED PORTION OR ALL OF THE INSTRUMENT SENSITIVITY TO LIE OUTSIDE THE SPECTRAL RANGE SPECIFIED///)  
704 FORMAT(///,1 34X_63HDETECTOR OMITTED BECAUSE SPECIFIED CENTER OF SLIT FUNCTION LIES OUTSIDE OF THE SPECIFIED SLIT FUNCTION///)  
705 FORMAT(///,1 34X_63HDETECTOR OMITTED BECAUSE UPPER SCAN LIMIT WAS INPUT LESS THAN OR EQUAL TO THE LOWER LIMIT///)

END
SUBROUTINE GROWTH

COMMON/CPLOT/LAMMIN,LAMMAX,DELLAM,NARRAY,CINT3,FACTRI(5)
COMMON/CARRAY/LAM(9000),ELAM(9000)
COMMON/CREAD/READ1,READ2,READ3,READ4,READ5,READ6
COMMON/CBAND1/ALPHAU,BETAU,CAPEU,CAPLU,DEEU,DEELU,RELU,TERMU
COMMON/CBAND2/WEU,WEUY,WEYU,WEZU,WEZUY,DEGENU,MU,ALNAT
COMMON/CTEMP/TELECT,TIV,TROT
COMMON/CWIDTH/WIDTHL,WIDTHV,RANGE
COMMON/CTRAN/PARTCC,NUBARO,Q_AOE,CINT1,CINT2,KMIN,KMAX
COMMON/CEXTRA/INDEX,NFILE_SYSTEM,TOTAL_OUTPUT(12)
REAL LAMI,LAM2,LAMMAX,LAMMIN,ILAH,ELAH,ILAMBDA,ELAMDA,ILAM3
DIMENSION DEPTHL(25),GROW(25)

LAMI= READ1
LAM2= READ2

C PRINT HEADING FOR CURVE-OF-GROWTH CALCULATION.
WRITE(6,600) LAMI,LAM2

C IF THE UPPER WAVELENGTH LIMIT WAS INPUT FIRST, WRITE AN ERROR
C MESSAGE AND Omit THIS CURVE OF GROWTH.
IF (LAM2 .LE. LAMI) GO TO 70

C IF WAVELENGTH LIMITS ARE OUTSIDE SPECTRAL RANGE CONSIDERED, SET
C INTEGRATION LIMITS TO APPROPRIATE END WAVELENGTH.
IF (LAMI .LT. LAMMIN) LAMI=LAMMIN
IF (LAM2 .GT. LAMMAX) LAM2=LAMMAX

C FIND INDICES IN INTENSITY ARRAY TO BE INCLUDED IN INTEGRATION.
NSTART= 1.0 + (LAMI-LAMMIN)/DELLAM
NEND= 1.0 + (LAM2-LAMMIN)/DELLAM

C DEFINE SPECIAL WAVELENGTHS NEEDED IN THE INTEGRATION.
COUNT = NSTART
LAMDA1= LAMMIN + (COUNT-1.0)*DELLAM
LAMDA2= LAMDA1 + DELLAM
COUNT = NEND
LAMDA3= LAMMIN + (COUNT-1.0)*DELLAM

C INITIALIZE DEPTH AND START CURVE-OF-GROWTH CALCULATION.
DEPTH= 3.162278E-7
M2=NEND
IF M2 .LE. NEND) M2=MEND+1
DO 60 M=1,25
DEPTH= DEPTH*3.162278
DO 10 M=NSTART,M2
IF (ELAM(M) .LE. 1.0E-36) GO TO 10
COUNT=M
LAMDBA= LAMMIN + (COUNT-1.0)*DELLAM
BLAM= 1.1904E-16*EXP(-1.43879/(LAMDBA*TELECT)/(LAMDBA**5)+(1.0-EXP(-1.43879/(LAMDBA*TELECT))))
ICILAM= ALOG((1.0-EXP(-1.43879/(LAMDBA*TELECT))))
ICILAM= ALOG((1.0-EXP(-1.43879/(LAMDBA*TELECT))))
ICILAM3= ALOG((1.0-EXP(-1.43879/(LAMDBA*TELECT))))
ICILAM4= ICILAM+ICILAM3+ICILAM+ICILAM
CILAM= ICILAM+ICILAM3+ICILAM+ICILAM
CONTINUE
10 CONTINUE

C TEST INTERVAL LIMITS.
IF (NSTART .LT. NEND) GO TO 20

C THE INTERVAL IS BOUNDED BY CONSECUTIVE ENTRIES IN THE LAMBDA ARRAY.
SLOPE= (LAMMIN+NARRAY)-DELLAM
SLOPE= (SLOPE*(LAM1-LAMDA1)+LAMMIN)+SLOPE*(LAM2-LAM1)/2.0E+4
GO TO 50

C IS THERE A RIGHT-HAND INCREMENT.
IF (NEND+EG-NARRAY) GO TO 30

C COMPUTE INTEGRATED INTENSITY FROM RIGHT-HAND INCREMENTAL AREA.
ILAMI = (ILAM(NEND) - ILAM(NEND+1)) * (LAM2 - LAMDA3) / 
(DELAM+ILAM(NEND))

TOTALI = (ILAMI+ILAM(NEND)) * (LAM2-LAMDA3) / 2.0E+4

C COMPUTE INTEGRATED INTENSITY FROM LEFT-HAND INCREMENTAL AREA.

30 ILAM1 = (ILAM(NSTART) - ILAM(NSTART+1)) * (LAMDA2 - LAM1) / 
(DELAM+ILAM(NSTART+1))

TOTAL1 = TOTAL1 + (ILAMI+ILAM(NSTART+1)) * (LAMDA2-LAM1) / 2.0E+4

C DO INTERVAL LIMITS BOUND A SINGLE ENTRY IN THE LAMBD Array.

IF (NEND .EQ. NSTART+1) GO TO 50

C COMPUTE INTEGRATED INTENSITY FROM CENTRAL INCREMENTAL AREAS.

NSTART = NSTART+2

DO 40 M = NSTART, NEND

40 TOTALI = TOTALI + (ILAM(M)+ILAM(M+1)) * DELAM / 2.0 E+4

C RESET NSTART FOR NEXT STEP OF DO LOOP ENDING AT STATEMENT 60.

NSTART = NSTART-2

50 DEPTH(M1) = DEPTH

60 GROW(M1) = TOTAL1

C WRITE CURVE-OF-GROWTH DATA.

WRITE(6,601) (DEPTH(M), GROW(M), M=1,251)

RETURN

C THERE IS AN ERROR IN THE LIMITS FOR THE INTEGRATION INTERVAL.

70 WRITE(6,700) LAM1, LAM2

RETURN

C FORMATS FOR WRITE STATEMENTS.

600 FORMAT(//)

1 5X,33HCURVE OF GROWTH CALCULATION FROM +F8.2x+M TO +F8.2+

2 10; ANGSTROMS/1

3 70X,10INTTEGRATED/

4 52X,9GEOMETRIC+9X+9INTENSITY/

5 52X,9DEPTH, CMx12WATTS/CW2-SR//)

601 FORMAT(2X,1PE9.3,10X,E9.3)

C FORMAT FOR ERROR STATEMENT.

700 FORMAT(//10X,16H THE LOWER LIMIT ,1PE11.4,3H IS GREATER THAN THE U
IPPER LIMIT ,1PE11.4,3H THEREFORE INTEGRATION WAS NOT PERFORMED. 1

END

******************************************************************************
SUBROUTINE ILAMDA

START

INITIALIZE -
EX(1) = λmin, EX(2) = λmax
EX(5001) = 0.0, EX(5002) = 0.0
NLAM = -1, NILAM = 4999
NOILAM = 0

READ READ1 TO READ6

READ6

WRITE HEADINGS

DO 30 M = 1, NLAM
30 WRITE EX(M), EX(M + 5000)

WRITE ERROR MESSAGE

NEWCASE = .TRUE.

RETURN
SUBROUTINE ONE

START
NSPRD0 = 1.1 + RANGE - WIDTH/\Delta a

CSPRD2 = ... 
CSPRD3 = ... 
CSPRD4 = ... 
CSPRD5 = ... 
SIGN = 1.0

\text{IF} \leq \text{CAPLL} \rightarrow \text{SIGN} = -1.0

SWITCH = 1
KU = KMIN
KL = KU + 1.0
BAND = 0.0

A

B
WRITE P BRANCH DATA

\text{SWITCH} = 2
KU = KMIN
KL = KU

A

C
WRITE Q BRANCH DATA

\text{SWITCH} = 3
KU = KMIN
KL = KU + 1.0

A

D
WRITE R BRANCH DATA

OR = ... 
APPROX = ... 

WRITE BAND, APPROX 
RETURN

SUBROUTINE ONE

A
BRANCH = 0.0

DO 90 M = KMIN, KMAX

\text{IF} \geq \lambda_{min} \rightarrow \text{BRANCH} = 0.0

\text{IF} \geq \lambda_{max} \rightarrow \text{BRANCH} = 0.0

\text{IF} \leq \lambda_{max} \rightarrow \text{BRANCH} = 0.0

\text{IF} \leq \lambda_{min} \rightarrow \text{BRANCH} = 0.0

\text{SWITCH} = 1

\text{SWITCH} = 2

\text{SWITCH} = 3

50

\text{FACTOR} = 1.0

ALTNAT = 0

KEXP = ... 
\text{FACTOR} = ... 

E = ... 

\text{NSCENT} = ... 
\text{NSTART} = ... 

\text{NSFART} = \geq 1 \rightarrow \text{NSSTART} = 1

\text{NEND} = ... 

\text{NEND} = \text{NARRAY} 

\text{NEND} = \text{NARRAY} 

\text{DO 70 M1 = NSTART, NEND}

\text{COUNT} = M1 

\lambda = \lambda_{min} + (\text{COUNT} - 1.0) \cdot \Delta a

E_{3}(\text{M1}) = ... 

\text{BRANCH} = \text{BRANCH} + E

80

\text{KU} = \text{KU} + 1.0

90

\text{KL} = \text{KL} + 1.0

\text{BAND} = \text{BAND} + \text{BRANCH}

\text{SYSTEM} = \text{SYSTEM} + \text{BRANCH}

A

\text{SWITCH} = 2

C

D

E
SUBROUTINE PRINT

WRITE HEADING

NEWCAS
TRUE
WRITE.E.O, NO, TRUE

FALSE
READ KIND

KIND
# LOG

WRITE HEADING

DO 10 M = 1, NARRAY

E_M = LOOIOIE_M/CI13

10

E_M0 = LOG_10(E_M) - CINT3

NWRITE = NARRAY/4
N1 = NWRITE + 1
N2 = 2*NWRITE + 1
N3 = 3*NWRITE + 1

DO 20 M = 1, NWRITE

WRITE SPECTRUM

20

N1 = N1 + 1
N2 = N2 + 1
N3 = N3 + 1

RETURN

WRITE HEADING

NWRITE = NARRAY/4
N1 = NWRITE + 1
N2 = 2*NWRITE + 1
N3 = 3*NWRITE + 1

DO 60 M = 1, NWRITE

WRITE SPECTRUM

60

N1 = N1 + 1
N2 = N2 + 1
N3 = N3 + 1

RETURN

WRITE HEADING

NWRITE = NARRAY/4
N1 = NWRITE + 1
N2 = 2*NWRITE + 1
N3 = 3*NWRITE + 1

DO 70 M = 1, NWRITE

WRITE SPECTRUM

70

N1 = N1 + 1

RETURN
SUBROUTINE INTRVL

START

WRITE HEADING

10

READ LAM1, LAM2

TOTAL1 = 0.0

LAM2 < LAM1

LAM1 < \lambda_{\text{min}}

LAM1 \geq \lambda_{\text{min}}

LAM1 < \lambda_{\text{max}}

LAM2 < \lambda_{\text{max}}

LAM1 \geq \lambda_{\text{min}}

LAM2 \geq \lambda_{\text{max}}

WRITE ERROR MESSAGE

70

NSTART = 1.0 + (LAM1 - \lambda_{\text{min}}) / \Delta \lambda

NEND = 1.0 + (LAM2 - \lambda_{\text{min}}) / \Delta \lambda

SLOPE = \ldots

TOTAL1 = \ldots

30

E_{\text{LAM1}} = \ldots

TOTAL1 = TOTAL1 + \ldots

NEND = NSTART + 1

NSTART = NSTART + 2

DO 40 M = NSTART, NEND

TOTAL1 = TOTAL1 + \ldots

40

WRITE INTEGRATION DATA

60

NINTRV = NINTRV - 1

\# 0

NINTRV

= 0

RETURN

66
SUBROUTINE GROWTH

START
LAMI = READI
LAM2 = READ2

WRITE HEADING

IF (LAMI < LMIN) THEN
  LAMI = LMIN
ELSE IF (LAMI > LMAX) THEN
  LAMI = LMAX
ENDIF

IF (LAM2 < LMIN) THEN
  LAM2 = LMIN
ELSE IF (LAM2 > LMAX) THEN
  LAM2 = LMAX
ENDIF

NSSTART = 1.0 + (LAMI - LMIN) / DX
NEND = 1.0 + (LAM2 - LMIN) / DX

COUNT = NSSTART

LAMDA1 = LMIN + (COUNT - 1.0) * DX
LAMDA2 = LAMDA1 + DX
COUNT = NEND

LAMDA3 = LMIN + (COUNT - 1.0) * DX

DEPTH = 3.162278 x 10^-7
M2 = NEND

DO 60 MI = 1, 25
TOTALI = 0.0
DEPTH = DEPTH x 3.162278
DO 10 M = NSSTART, M2
  IF (E(M) < 10^-36) THEN
    CONTINUE
  ELSE
    IF (LAM(M) - NMIN / NINT3 - I) EX(M) = ILI
    I = (LAM(M) - NMIN / NINT3 - I) / LAM(M)
  ENDIF
  TOTALI = TOTALI + M2 - NEND + 1
  SLOPE = NSSTART + I - NSTART
  TOTALI = TOTALI + M2 - NEND + 1
  WRITE GROWTH DATA
  WRITE ERROR MESSAGE

RETURN
**APPENDIX C**

**DESCRIPTION OF INPUT CARDS FOR PROGRAM**

<table>
<thead>
<tr>
<th>Card number</th>
<th>Columns</th>
<th>Format</th>
<th>Content</th>
<th>Number of cards per case</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1-4</td>
<td>A4</td>
<td>Case card</td>
<td>1</td>
<td>Columns 1-4 must spell CASE. The remaining spaces may be used for data deck identification. This card is read in the main program.</td>
</tr>
<tr>
<td>2</td>
<td>1-72</td>
<td>12A6</td>
<td>Title card</td>
<td>3</td>
<td>Any 72 alphanemic characters may be written in the first 72 spaces of each card. The information input on these cards will be written on the header of each case. These cards are read in the main program.</td>
</tr>
<tr>
<td>3</td>
<td>1-10</td>
<td>E10.0</td>
<td>Spectral coverage and resolution</td>
<td>1</td>
<td>((\text{LAMMAX}-\text{LAMMIN})/\Delta \text{LAM} &lt; 8999.) \newline This card is read in the main program.</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>(\text{LAMMIN}, \lambda_{\text{min}})</td>
<td>(\text{LAMMAX}, \lambda_{\text{max}})</td>
<td>(\Delta \lambda)</td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>E10.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>1-10</td>
<td>E10.0</td>
<td>Incident spectrum</td>
<td>0-2000</td>
<td>(\text{LAM}(1) \leq \text{LAMMIN}, \text{LAM}(\text{LAST}) \geq \text{LAMMAX}) \newline (\text{LAM}(M) &lt; \text{LAM}(M+1)) \newline Blank cards are not required if an incident spectrum is not specified. Maximum number of points permitted is 2000. The last card can have only one point, if desired. If the final output is to be a curve of growth or an optically thin spectrum, an incident spectrum should not be specified. These cards are read in subroutine ILAMDA.</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>(\text{LAM}(M), \lambda)</td>
<td>(\text{ILAM}(M), I_{\lambda})</td>
<td></td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>E10.0</td>
<td>(\text{LAM}(M+1))</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>31-40</td>
<td>E10.0</td>
<td>(\text{ILAM}(M+1))</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Card number</td>
<td>Columns</td>
<td>Format</td>
<td>Content</td>
<td>Number of cards per band system</td>
<td>Comments</td>
</tr>
<tr>
<td>-------------</td>
<td>---------</td>
<td>--------</td>
<td>-------------------</td>
<td>---------------------------------</td>
<td>--------------------------------------------------------------------------</td>
</tr>
<tr>
<td>BAND SYSTEM CARDS: Two alternatives - Band system can be input from magnetic tape or from cards. Band systems input from magnetic tape</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>1-10</td>
<td>E10.0</td>
<td>Band system data and name</td>
<td>1</td>
<td>Any number of band systems can be included in a layer or a case.</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>PARTCC, N</td>
<td></td>
<td>Name must be left justified and must be exactly one of the following:</td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>E10.0</td>
<td>TELECT, Tel ect</td>
<td></td>
<td>CNeVbb, CNeRED, CNe4+b, CH4300</td>
</tr>
<tr>
<td></td>
<td>31-40</td>
<td>E10.0</td>
<td>TVIB, Tvib</td>
<td></td>
<td>C2SWAN, N2b60, N2+b-l, BB-X</td>
</tr>
<tr>
<td></td>
<td>67-72</td>
<td>A6</td>
<td>TROT, Trot</td>
<td></td>
<td>C0ASDI, C2PHIL, N2bL+b, N0bBbb</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>NAME</td>
<td></td>
<td>C2bSb, 262+b, N2LBH, CH3900</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>b = blank space. This card is read in the main program, subroutine ILAMDA, or subroutine ATOMIC.</td>
</tr>
<tr>
<td>5-a</td>
<td>1-10</td>
<td>E10.0</td>
<td>Band system data and name</td>
<td>1</td>
<td>Any number of band systems can be included in a layer or a case.</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>PARTCC, N</td>
<td></td>
<td>Name can be any A6 identifier.</td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>E10.0</td>
<td>TELECT, Tel ect</td>
<td></td>
<td>IF CAPLU - CAPLL = 0 INDEX = 1.0</td>
</tr>
<tr>
<td></td>
<td>31-40</td>
<td>E10.0</td>
<td>TVIB, Tvib</td>
<td></td>
<td>IF CAPLU - CAPLL = ±1 and this is not a 2π → 2Σ (or vice versa) transition</td>
</tr>
<tr>
<td></td>
<td>41-45</td>
<td>F5.0</td>
<td>INDEX</td>
<td></td>
<td>INDEX = 2.0. If this is a 2π → 2Σ (or vice versa) transition INDEX = 3.0.</td>
</tr>
<tr>
<td></td>
<td>67-72</td>
<td>A6</td>
<td>NAME</td>
<td></td>
<td>This card is read in the main program, subroutine ILAMDA, or subroutine ATOMIC.</td>
</tr>
<tr>
<td>Card number</td>
<td>Columns</td>
<td>Format</td>
<td>Content</td>
<td>Number of cards per band system</td>
<td>Comments</td>
</tr>
<tr>
<td>-------------</td>
<td>---------</td>
<td>--------</td>
<td>----------------------------------------------</td>
<td>---------------------------------</td>
<td>-----------------------------------------------------------</td>
</tr>
<tr>
<td>5-b</td>
<td>1-10</td>
<td>E10.0</td>
<td>Band system data</td>
<td>1</td>
<td>This card is read in subroutine SETUP.</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>LEVELS</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>E10.0</td>
<td>MU, ( \mu_A )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>31-40</td>
<td>E10.0</td>
<td>DEL, ( D_e )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>41-50</td>
<td>E10.0</td>
<td>REL, ( r_e )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>51-60</td>
<td>E10.0</td>
<td>DZEROL, ( D_0 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>61-70</td>
<td>E10.0</td>
<td>CAPAU, ( A' )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>71-80</td>
<td>E10.0</td>
<td>CAPLU, ( \Lambda' )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5-c</td>
<td>1-10</td>
<td>E10.0</td>
<td>Band system data</td>
<td>1</td>
<td>This card is read in subroutine SETUP.</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>NUSPIN, ( I )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>E10.0</td>
<td>DEL, ( D_e )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>31-40</td>
<td>E10.0</td>
<td>BETAL, ( \beta''_e )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>41-50</td>
<td>E10.0</td>
<td>REL, ( r_e )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>51-60</td>
<td>E10.0</td>
<td>DZEROL, ( D_0 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>61-70</td>
<td>E10.0</td>
<td>CAPAL, ( A'' )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>71-80</td>
<td>E10.0</td>
<td>CAPLL, ( \Lambda'' )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5-d</td>
<td>1-10</td>
<td>E10.0</td>
<td>Spectroscopic constants</td>
<td>LEVELS</td>
<td>The appropriate cards for the upper and lower levels of the transition must be input first and second, respectively. These cards are read in subroutine SETUP.</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>DEGEN(M), ( \bar{d} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>E10.0</td>
<td>TERM(M), ( T_e )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>31-40</td>
<td>E10.0</td>
<td>( \omega_e )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>41-50</td>
<td>E10.0</td>
<td>( \omega_e x_e )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>51-60</td>
<td>E10.0</td>
<td>( \omega_e y_e )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>61-70</td>
<td>E10.0</td>
<td>( \omega_e z_e )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>71-80</td>
<td>E10.0</td>
<td>( \alpha_e )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Card number</td>
<td>Columns</td>
<td>Format</td>
<td>Content</td>
<td>Number of cards per band system</td>
<td>Comments</td>
</tr>
<tr>
<td>-------------</td>
<td>---------</td>
<td>--------</td>
<td>-----------------------------------</td>
<td>--------------------------------</td>
<td>----------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>6</td>
<td>1-10</td>
<td>E10.0</td>
<td>VU, v'</td>
<td>Any number</td>
<td>Cards 6 and 7 specify one vibrational band. Any number of bands may be input and these must follow card number 5 if the band system is input from tape, or 5-d if the input is from cards. KMIN and KMAX may be left blank. If KMIN is left blank, it will be set to 2. If KMAX is left blank and a value for DZEROU and/or DZEROL is known, KMAX will be computed; otherwise KMAX will be set to 150. This card is read in the main program.</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>VL, v''</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>E10.0</td>
<td>KMIN, Kmin</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>31-40</td>
<td>E10.0</td>
<td>KMAX, Kmax</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>1-10</td>
<td>E10.0</td>
<td>( \sum_2 \left( \frac{1}{e_n} \right) )</td>
<td>Any number</td>
<td>NUBARO and RANGE may be left blank. If NUBARO is left blank, its value will be computed from the spectroscopic constants. If RANGE is left blank, it will be set to 5 if WIDTHL ( \neq 0 ); if WIDTHL = 0, RANGE will be set to 3. FRANCK may be left blank for a band system input from tape. If this is done, the value stored on tape is used in the calculation. This card is read in subroutine VU VL.</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>WIDTHL, ( w_e )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>E10.0</td>
<td>WIDTHHL, ( w_l )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>31-40</td>
<td>E10.0</td>
<td>NUBARO, ( \tilde{v}_o(v', v'') )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>41-50</td>
<td>E10.0</td>
<td>FRANCK, ( q_{v', v''} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>51-60</td>
<td>E10.0</td>
<td>RANGE</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Card number</td>
<td>Columns</td>
<td>Format</td>
<td>Content</td>
<td>Number of cards per atomic system</td>
<td>Comments</td>
</tr>
<tr>
<td>-------------</td>
<td>---------</td>
<td>--------</td>
<td>--------------</td>
<td>-----------------------------------</td>
<td>-----------------------------------------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Atomic system cards</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>1-10</td>
<td>E10.0</td>
<td>ATOMCC, N</td>
<td>1</td>
<td>NAME can be any A6 identifier. Any number of atomic systems can be specified for each layer and they can be mixed with the specified band systems. However, the printed output will be easier to read if all the atomic systems are either input before or after the band systems. This card is read either in the main program, subroutine ILAMDA, or ATOMIC.</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>T I E L C T,</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>E10.0</td>
<td>Q, Q</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>67-72</td>
<td>A6</td>
<td>NAME</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>1-10</td>
<td>E10.0</td>
<td>Atomic data</td>
<td>Any number following each card 8</td>
<td>RANGE may be left blank. If this is done and WIDTHL ≠ 0, RANGE is set to 5; otherwise, RANGE is set to 3. This card is read in subroutine ATOMIC.</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>WIDTHL, Wg</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>E10.0</td>
<td>DEGENU, d'</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>31-40</td>
<td>E10.0</td>
<td>TERMU, T_e</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>41-50</td>
<td>E10.0</td>
<td>EINSTEIN, A_{ul}</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>51-60</td>
<td>E10.0</td>
<td>LAMCL, λ_{e}</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>61-66</td>
<td>E6.0</td>
<td>RANGE</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Card number</td>
<td>Columns</td>
<td>Format</td>
<td>Content</td>
<td>Number of cards per case</td>
<td>Comments</td>
</tr>
<tr>
<td>-------------</td>
<td>---------</td>
<td>--------</td>
<td>------------------------------</td>
<td>--------------------------</td>
<td>------------------------------------------------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Curve-of-growth</td>
<td></td>
<td>LAM1 &lt; LAM2, LAM1 &gt; LAMMIN, LAM2 ≤ LAMMAX</td>
</tr>
<tr>
<td>10</td>
<td>1-10</td>
<td>E10.0</td>
<td>LAM1, λ</td>
<td></td>
<td>This card specifies that a curve-of-growth will be printed on the output sheet. The card must follow the last vibrational band or atomic line card. Any number of integration intervals LAM1 to LAM2 may be specified, and the word GROWTH must appear on each card. Blank cards are not required if a curve of growth is not needed. A curve-of-growth calculation can be specified for any single-layer case or for the first layer of a multilayer case. However, if an incident spectrum is specified, it will not be used and, in fact, will be re-initialized to zero. This card is read in the main program or subroutine ATOMIC.</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>LAM2, λ</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>67-72</td>
<td>A6</td>
<td>GROWTH</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Any number</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Card number</th>
<th>Columns</th>
<th>Format</th>
<th>Content</th>
<th>Number of cards per case</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>1-10</td>
<td>E10.0</td>
<td>DEPTH, l, x</td>
<td></td>
<td>LAYER must be left-justified. If the &quot;true&quot; spectrum for a given incident spectrum and geometric DEPTH is to be computed, this card must be input with the word LAYER written as indicated. This card follows the last curve-of-growth card. If a &quot;true&quot; spectrum is not to be computed, and the final output is to be for an optically thin spectrum, this card is omitted. This card is read in the main program or subroutine ATOMIC.</td>
</tr>
<tr>
<td></td>
<td>67-72</td>
<td>A6</td>
<td>LAYER</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>One for each layer</td>
<td></td>
</tr>
<tr>
<td>Card number</td>
<td>Columns</td>
<td>Format</td>
<td>Content</td>
<td>Number of cards per case</td>
<td>Comments</td>
</tr>
<tr>
<td>-------------</td>
<td>---------</td>
<td>--------</td>
<td>---------</td>
<td>-------------------------</td>
<td>----------</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Print spectrum cards</td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>67-72</td>
<td>A6</td>
<td>Specification of whether or not spectrum is to be printed.</td>
<td>1</td>
<td>OUTPUT must be left-justified.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>OUTPUT</td>
<td></td>
<td>1. To print the spectrum, OUTPUT = PRINT.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2. To not print the spectrum, OUTPUT = NONE. This card is read in subroutine ATOMIC or the main program.</td>
</tr>
<tr>
<td>13</td>
<td>67-72</td>
<td>A6</td>
<td>Specification of type of printed output</td>
<td>0 or 1</td>
<td>KIND must be left-justified.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>KIND</td>
<td></td>
<td>1. If it is desired to print log _{10} (intensity), KIND = LOG</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2. If it is desired to print intensity directly, KIND is left blank. This card is required only if a printed spectrum was specified on card 12. This card is read in subroutine PRINT.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Number of intervals and slits card</td>
<td></td>
<td></td>
<td></td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>1-5</td>
<td>I5</td>
<td>Specification of number of intervals and slits</td>
<td></td>
<td>If no intervals or slits are desired, a blank card must be included, and it will be the last card in the case. This card is read in the main program.</td>
</tr>
<tr>
<td></td>
<td>6-10</td>
<td>I5</td>
<td>NINITR</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>NSLIT</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Interval cards</td>
<td></td>
<td></td>
<td></td>
<td>NINITR</td>
<td>LAM1 &lt; LAM2</td>
</tr>
<tr>
<td>15</td>
<td>1-10</td>
<td>E10.0</td>
<td>Integration limits for interval.</td>
<td></td>
<td>LAM1 ≥ LAMMIN, LAM2 ≤ LAMMAX</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>LAM1, λ</td>
<td></td>
<td>These cards must follow card 14.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>LAM2, λ</td>
<td></td>
<td>These cards are read in subroutine INTRVL.</td>
</tr>
<tr>
<td>Card number</td>
<td>Columns</td>
<td>Format</td>
<td>Content</td>
<td>Number of cards per slit case</td>
<td>Comments</td>
</tr>
<tr>
<td>-------------</td>
<td>---------</td>
<td>--------</td>
<td>------------------</td>
<td>------------------------------</td>
<td>----------</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Slit cards: There are four types of slits and any number of each may be specified for each case. The total number of SLITS must be equal to NSLIT. The slit types are: (a) fixed Gaussian, (b) fixed linear, (c) scanning Gaussian, and (d) scanning linear.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(a) Fixed Gaussian slit cards</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>16-a</td>
<td>1-4</td>
<td>A4</td>
<td>Slit identification</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>SLIT</td>
<td>1</td>
<td>The first four columns of this card must spell SLIT. The remaining columns can contain any desired information. This card is read in subroutine SLIT.</td>
</tr>
<tr>
<td>17-a</td>
<td>1-5</td>
<td>I5</td>
<td>NPOINT</td>
<td>1</td>
<td>NPOINT = 0 (or blank) for this slit case. This card is read in subroutine SLIT.</td>
</tr>
<tr>
<td>18-a</td>
<td>1-10</td>
<td>E10.0</td>
<td>LAMCL</td>
<td>1</td>
<td>LAMCL ± 3.0(WIDTH) must fall between LAMMAX and LAMMIN. LAMCL = spectral location of slit center. RLAMCL = peak value of instrument sensitivity. WIDTH = width of slit at half-peak sensitivity. This card is read in subroutine SLIT.</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>RLAMCL</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>E10.0</td>
<td>WIDTH</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(b) Fixed linear slit cards</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>16-b</td>
<td>1-4</td>
<td>A4</td>
<td>Slit identification</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>SLIT</td>
<td>1</td>
<td>The first four columns of this card must spell SLIT. The remaining columns can contain any desired information. This card is read in subroutine SLIT.</td>
</tr>
<tr>
<td>17-b</td>
<td>1-5</td>
<td>I5</td>
<td>NPOINT</td>
<td>1</td>
<td>NPOINT ≤ 100 and LAMS1 must not allow any part of the instrument sensitivity to fall outside the computed spectrum. This card is read in subroutine SLIT.</td>
</tr>
<tr>
<td></td>
<td>25-34</td>
<td>E10.0</td>
<td>LAMS1</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

1LAMS1 = spectral location at which slit function will be centered.
<table>
<thead>
<tr>
<th>Card number</th>
<th>Columns</th>
<th>Format</th>
<th>Content</th>
<th>Number of cards per slit case</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>18-b</td>
<td>1-10</td>
<td>E10.0</td>
<td>Slit function</td>
<td></td>
<td>The slit function abscissa must be in Å, but they can be relative to any origin desired. The slit function abscissa must be in Å, but they can be relative to any origin desired. LAM(M) &lt; LAM(M + 1)</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>LAM(M)</td>
<td></td>
<td>These cards are read in subroutine SLIT.</td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>E10.0</td>
<td>RSLIT(M)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>31-40</td>
<td>E10.0</td>
<td>RSLIT(M + 1)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>41-50</td>
<td>E10.0</td>
<td>LAM(M + 2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>51-60</td>
<td>E10.0</td>
<td>RSLIT(M + 2)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

19-b Slit function data

<table>
<thead>
<tr>
<th>Card number</th>
<th>Columns</th>
<th>Format</th>
<th>Content</th>
<th>Number of cards per slit case</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1-10</td>
<td>E10.0</td>
<td>LAMCL</td>
<td>1</td>
<td>LAMCL = position in slit function to be located at LAMS1. Rlamcl = calibration factor. The instrument sensitivity is given by the product Rlamcl Rslit(M). LAM(1) ≤ LAMCL ≤ LAM(NPOINT)</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>Rslamcl</td>
<td></td>
<td>This card is read in subroutine SLIT.</td>
</tr>
</tbody>
</table>

(c) Scanning Gaussian slit cards

<table>
<thead>
<tr>
<th>Card number</th>
<th>Columns</th>
<th>Format</th>
<th>Content</th>
<th>Number of cards per slit case</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>16-c</td>
<td>1-4</td>
<td>A4</td>
<td>Slit identification</td>
<td></td>
<td>The first four columns of this card must spell SLIT. The remaining columns can contain any desired information. This card is read in subroutine SLIT.</td>
</tr>
<tr>
<td></td>
<td>1-5</td>
<td>I5</td>
<td>NPOINT</td>
<td></td>
<td>NPOINT = 0, SCAN = 1, STEP = distance between steps in SCAN, LAMS1 = starting wavelength of SCAN, LAMS2 = stopping wavelength of SCAN, NRLAMS = number of pairs of values specifying the spectral calibration of the instrument.</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>I1</td>
<td>SCAN</td>
<td></td>
<td>LAMS1 ≥ LAMMIN + 3.0(WIDTH) LAMS2 ≤ LAMMAX - 3.0(WIDTH) This card is read in subroutine SLIT.</td>
</tr>
<tr>
<td></td>
<td>15-24</td>
<td>E10.0</td>
<td>STEP</td>
<td></td>
<td>This card is read in subroutine SLIT.</td>
</tr>
<tr>
<td></td>
<td>25-34</td>
<td>E10.0</td>
<td>LAMS1</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>35-44</td>
<td>E10.0</td>
<td>LAMS2</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>46-50</td>
<td>I5</td>
<td>NRLAMS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>18-c</td>
<td>21-30</td>
<td>E10.0</td>
<td>WIDTH</td>
<td>1</td>
<td>WIDTH = width of slit function at half-peak height. This card is read in subroutine SLIT.</td>
</tr>
<tr>
<td>Card number</td>
<td>Columns</td>
<td>Format</td>
<td>Content</td>
<td>Number of cards per slit case</td>
<td>Comments</td>
</tr>
<tr>
<td>-------------</td>
<td>---------</td>
<td>--------</td>
<td>---------</td>
<td>-------------------------------</td>
<td>----------</td>
</tr>
<tr>
<td>19-c</td>
<td>1-10</td>
<td>E10.0</td>
<td>Spectral calibration</td>
<td>Enough to specify the instrument sensitivity at any wavelength along the scan is given by the spectral calibration at the slit function center. Interpolated values of the spectral calibration are used when appropriate.</td>
<td>LAMR(M) &lt; LAMR(M + 1) LAMR(1) ≤ LAMSL1, LAMR(NRLAMS) ≥ LAMS2.</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>LAMR(M)</td>
<td>NRLAMS</td>
<td></td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>E10.0</td>
<td>LAMR(M + 1)</td>
<td>pairs of slit function data points</td>
<td></td>
</tr>
<tr>
<td></td>
<td>31-40</td>
<td>E10.0</td>
<td>LAMR(M + 1)</td>
<td>spectral calibration</td>
<td></td>
</tr>
<tr>
<td></td>
<td>41-50</td>
<td>E10.0</td>
<td>LAMR(M + 2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>51-60</td>
<td>E10.0</td>
<td>LAMR(M + 2)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(d) Scanning linear slit cards

<table>
<thead>
<tr>
<th>Card number</th>
<th>Columns</th>
<th>Format</th>
<th>Content</th>
<th>Number of cards per slit case</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>16-d</td>
<td>1-4</td>
<td>A4</td>
<td>Slit identification</td>
<td>1</td>
<td>The first four columns of this card must spell SLIT. The remaining columns can contain any desired information. This card is read in subroutine SLIT.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>SLIT</td>
<td></td>
<td></td>
</tr>
<tr>
<td>17-d</td>
<td>1-5</td>
<td>I5</td>
<td>Slit data</td>
<td>1</td>
<td>NPOINT ≤ 100. All other comments made for card 17-c of the scanning Gaussian slit apply here as well. This card is read in subroutine SLIT.</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>I1</td>
<td>SCAN</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>15-24</td>
<td>E10.0</td>
<td>STEP</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>25-34</td>
<td>E10.0</td>
<td>LAMS1</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>35-44</td>
<td>E10.0</td>
<td>LAMS2</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>46-50</td>
<td>I5</td>
<td>NRLAMS</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Card number</th>
<th>Columns</th>
<th>Format</th>
<th>Content</th>
<th>Number of cards per slit case</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>18-d</td>
<td>1-10</td>
<td>E10.0</td>
<td>Slit function</td>
<td>Enough to specify but they can be relative to any origin desired.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>LAMR(M)</td>
<td>NPOINT</td>
<td></td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>E10.0</td>
<td>LAMR(M + 1)</td>
<td>pairs of slit function data points</td>
<td></td>
</tr>
<tr>
<td></td>
<td>31-40</td>
<td>E10.0</td>
<td>LAMR(M + 1)</td>
<td>spectral calibration</td>
<td></td>
</tr>
<tr>
<td></td>
<td>41-50</td>
<td>E10.0</td>
<td>LAMR(M + 2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>51-60</td>
<td>E10.0</td>
<td>LAMR(M + 2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Card number</td>
<td>Columns</td>
<td>Format</td>
<td>Content</td>
<td>Number of cards per slit case</td>
<td>Comments</td>
</tr>
<tr>
<td>------------</td>
<td>---------</td>
<td>--------</td>
<td>--------------------------</td>
<td>------------------------------</td>
<td>----------</td>
</tr>
<tr>
<td>19-d</td>
<td>1-10</td>
<td>E10.0</td>
<td>Slit function data</td>
<td>1</td>
<td>LAMCL = position in the slit function that locates the slit during each step of the scan. LAM(1) ≤ LAMCL ≤ LAM(NPOINT) This card is read in subroutine SLIT.</td>
</tr>
<tr>
<td>20-d</td>
<td>1-10</td>
<td>E10.0</td>
<td>Spectral calibration</td>
<td>Enough to specify</td>
<td>Comments for card number 19-c in the scanning Gaussian case apply here as well.</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>E10.0</td>
<td>LAM(M)</td>
<td>NRLAMS pairs</td>
<td></td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>E10.0</td>
<td>LAM(M + 1)</td>
<td>of spectral calibration</td>
<td></td>
</tr>
<tr>
<td></td>
<td>31-40</td>
<td>E10.0</td>
<td>LAM(M + 1)</td>
<td>calibration points</td>
<td></td>
</tr>
<tr>
<td></td>
<td>41-50</td>
<td>E10.0</td>
<td>LAM(M + 2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>51-60</td>
<td>E10.0</td>
<td>RIAM(M + 2)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
APPENDIX D

LISTING OF SPECTROSCOPIC CONSTANTS AND FRANCK-CONDON FACTORS
FOR MOLECULAR BAND SYSTEMS ON MAGNETIC TAPE

In the listing of the Franck-Condon factors, values of 0.0 are printed as a row of stars (*).
<table>
<thead>
<tr>
<th>STATE</th>
<th>SPIN</th>
<th>QUANTUM NUMBER OF</th>
<th>ROTATIONAL CONSTANT DE, I/CM</th>
<th>ELECTRONIC DEGENERACY</th>
<th>ELECTRONIC ENERGY WE</th>
<th>ELECTRONIC WEIGHT</th>
<th>ALPHA</th>
</tr>
</thead>
<tbody>
<tr>
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**Franck-Condon Factors**

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**Spectrographic Constants for A and X States from McElroy and Rigotti,**


STATE DATA FROM HERZBERG EXCEPT WE AND WE0 WHICH WERE TAKEN FROM


**DISSOCIATION ENERGIES BASED ON HERZBERG P.455 AND ADJUSTED TO 8.2 EV.**

*THIS TRANSITION OCCURS IN SUBROUTINE ZERO.*
Table 1: Spectroscopic Constants for A and X States from Peletto and Riggutt's Work

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<th>LINE</th>
<th>ALTERNATION</th>
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<th>SPIN</th>
<th>COUPLING</th>
<th>QUANTUM NUMBER</th>
<th>RESULTANT ELECTRONIC ANGULAR MOMENTUM</th>
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**Notes:**
- Spectroscopic constants for A and X states from Peletto and Riggutt's work.
- States data from Herzberg except where noted.
- Spin coupling constant A taken from Herzberg which is close to average value by Peletto and Riggutt's work.
- This transition computed in subroutine S2 PE2.
### Spectrographic Constants from Ballik and Ramsay Astrophys. J., 137, 1963

Except for spin coupling constants which were taken from Herzberg.


This transition computed in subroutine ZEO.

#### Table 1: Spectrographic Constants

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#### Table 2: Calculation of Transition Energy

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#### Table 4: FRANCK-CONDON FACTORS

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84
SPECTROSCOPIC CONSTANTS FROM HERZBERG.
MORSE FRANCK–CONDON FACTORS ASTROPHYS 4, P 55 (1955)
THIS TRANSITION COMPUTED IN SUBROUTINE $32 P I 2$.

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- **WEYE**
- **BE**
- **CI**
- **CI**
- **CI**
- **CI**
- **CI**

**SECTRACO COASTANTS FROM HERBERG**

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**SPECTROGRAPHIC CONSTANTS FROM HERZBERG.**

**AVERAGE VALUES OF PI 1/2 AND PI 3/2 IN APPROPRIATE PLACES.**

**RKR FRANCK-CASERSON FACTORS JQSRT VOl. 4 P271 1964**

**THIS TRANSITION COMPUTED IN SUBROUTINE S2 PI2**
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### List

- **COASDI** stands for CO ASLNE BANDS. SPECTROGRAPHIC CONSTANTS FROM ERZBERG.
- Morse FRANK-COLOID FACTORS BY JARMAIN, FRASER, AND NICHOLLS.
- This transition CCPUCED IN SUBROUTINE ONE.

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|-----------|----------------------------------------|-----------------|-----------------|
| G         | 0.0                                    | 12              | **              |

### Equations

1. \[ E_{\text{upper}} = E_{\text{lower}} + \Delta E \]
2. \[ \Delta E = \frac{1}{2} \sum J(J+1) \]
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**Notes:**
- C2PHIL STANDS FOR C2 PHILLIPS BANDS.
- SPECTROGRAPHIC CONSTANTS FROM BALLIK AND RANSAY ASTROPHYS J 137 1963 P84.
- FOR FRANKC-CCCON FACTORS JCSMT VOL 5 1965 P 165.
- TRANSITION COMPUTED IN SUBROUTINE CNE.
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**Notes:**
- The table lists transitions computed in subroutine ZERC.
- The transitions are specified for atomic levels with reduced nuclear spin numbers.
- The table includes electronic factors for molecules and levels.
- The dissociation constants and internuclear distances are also listed.

**Reference:**
- SPECTROGRAPHIC CONSTANTS FROM HERZBERG.
- MORSE FRANCK-CONDON FACTORS BY JARMAN, FRASER, AND NICHOLLS 1954.
- ASTROP HYS J 122, 55 (1953).

**Additional Data:**
- Reduced atomic weight
- Nuclear spin numbers
- Electron coupling constants
- Quantum number changes
- Rotational energy constants
- Electronic term factors
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97
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MCSE FRANCK-CONDON FACTORS JOSBT VOL 1 1609 1867.


THIS TRANSITION COMPUTED IN SUBROUTINE ZERO.

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SPECTROSCOPIC CONSTANTS FROM HERZBERG.
MORSE FRANCK-CONDON FACTORS BY JARMAIN, FRASER, AND NICHOLLS 1954
ASTROPHYS J 122, 55 (1955)
THIS TRANSITION COMPUTED IN SLOMOLINE S2 PI2.

<table>
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<table>
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<th>NUMBER SPECIFYING</th>
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<tbody>
<tr>
<td>3</td>
<td>SPECIFYING DATA LOCATION</td>
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<tr>
<td>18</td>
<td>CN TAPE</td>
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SPECTROSCOPIC CONSTANTS FROM HERZBERG.
MORSE FRANCK-CONDON FACTORS BY JARMAIN, FRASER, AND NICHOLLS 1954
ASTROPHYS J 122, 55 (1955)
THIS TRANSITION COMPUTED IN SLOMOLINE S2 PI2.
APPENDIX E

SAMPLE CASE
### Sample Case for NASA TN

**Calculation includes** the (1010) band of the CN red system. 2 atomic nitrogen lines and an instrument calibration.

**The spectrum comprised from 10600.00 to 11085.00 Angstroms at 0.025 Angstrom intervals.**

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<td>VIBRATIONAL TEMPERATURE DEGREES K</td>
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**Spin Coupling Constant** (K) for Resultant Electronic Angular Momentum about Internuclear Axis:

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<th>K</th>
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**Electronic Degeneracy** (K)

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**Vibrational Quantum Number** (K)

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**Transition Moment** (K)

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<th>IN LINE</th>
<th>WIDTH AT HALF-HEIGHT</th>
<th>GAUSS LORENTZ FACTOR</th>
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<tr>
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**Wavelength Intensity** (K) in Angstroms/W/cm²-micron-SR

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<th>WAVELENGTH</th>
<th>INTENSITY</th>
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</thead>
<tbody>
<tr>
<td>11042.79</td>
<td>2.2049E-03</td>
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**Atomic Line Spectrum for N**

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**Wavelength in Angstroms**

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<thead>
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<th>INTENSITY</th>
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<tbody>
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**System Total of All Integrated Intensities**

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<thead>
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<th>INTENSITY</th>
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</thead>
<tbody>
<tr>
<td>9.2552E 02</td>
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</tr>
</tbody>
</table>

**This is a radiative transport solution, depth of above radiating layer is 1.00 cm.**

**Tabulation of Computed Spectrum**

<table>
<thead>
<tr>
<th>WAVELENGTH</th>
<th>INTENSITY</th>
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<tbody>
<tr>
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<tr>
<td>11042.82</td>
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<tr>
<td>11042.87</td>
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102
DETECTOR OUTPUT SIGNAL GIVEN BY A SPECIFIED INSTRUMENT RESPONSE

-------------------------------
SPECTROGRAPH OR SCANNING SPECTROMETER 1
SPECTRAL RANGE FROM 10865.50 TO 11079.50 ANGSTROMS COMPUTED AT 0.250 ANGSTROM INTERVALS
SLIT FUNCTION SPECIFIED BY LINEAR SEGMENTS

<table>
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<th>SLIT ANGSTROMS FUNCTION</th>
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<tr>
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SPECTRAL CALIBRATION OF INSTRUMENT THAT MULTIPLIES SLIT FUNCTION TO YIELD INSTRUMENT SENSITIVITY

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LOCATION OF INSTRUMENT OUTPUT

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<th>$^2\Pi \rightarrow ^2\Sigma$</th>
<th>$^{2}\Sigma \rightarrow ^{2}\Pi$</th>
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<td>+1</td>
<td>+1</td>
</tr>
<tr>
<td>$R_1$</td>
<td>$S_1$</td>
<td>-1</td>
<td>-1</td>
<td>+1</td>
</tr>
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<td>$S_{R_{21}}$</td>
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<td>-1</td>
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<td>$O_{P_{12}}$</td>
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<td>+1</td>
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<td>$S_2$</td>
<td>+1</td>
<td>+1</td>
<td>-1</td>
</tr>
<tr>
<td>$Q_{P_{21}}$</td>
<td>$Q_{R_{12}}$</td>
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<td>+1</td>
<td>-7</td>
</tr>
<tr>
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<td>$S_2$</td>
<td>-1</td>
<td>-1</td>
<td>+1</td>
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<td>$Q_{R_{12}}$</td>
<td>$Q_{P_{21}}$</td>
<td>(same NUBAR as $Q_1$)</td>
<td>-1</td>
<td>+1</td>
</tr>
<tr>
<td>$R_2$</td>
<td>$S_1$</td>
<td>+1</td>
<td>+1</td>
<td>+1</td>
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<td>$R_{Q_{21}}$</td>
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<td>(same NUBAR as $R_2$ or $P_2$)</td>
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<td>+1</td>
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<td>-1</td>
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<td>$P_{Q_{12}}$</td>
<td>$R_{Q_{21}}$</td>
<td>(same NUBAR as $P_1$ or $R_1$)</td>
<td>+1</td>
<td>-1</td>
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</table>
Figure 1.- Simplified flow chart of Main Program.
Figure 2.- Illustration of notation used in building the spontaneous-emission spectrum.
Figure 3.- Effective potential curves of HgH in the ground state. (Reproduced from ref. 9)
Figure 4.- Expressions used to find internuclear distance $R'$, at the local maximum of the potential well.

\[ f(R) = R^3 \left[ 1 - e^{-\beta (R - R_e)} \right] e^{-\beta (R - R_e)} \]

\[ g(K) = \frac{h K (K+1)}{8\pi^2 c_\mu D_e \beta} \]

Minimum of potential well

Local maximum of potential well, $R'$

(R - $R_e$), cm

(R - $R_e$), cm
Figure 5.- Energy difference between local maximum of potential well and sum of vibrational and rotational energies.
Figure 6. - Computed spectrum with integration limits.
(a) Gaussian slit function.  
(b) Linear-segment slit function.

Figure 7.- Slit functions used in program.
Figure 8.- Spectral calibration of grating spectrograph or scanning spectrometer.
Figure 9.- Illustration of integration to produce instrument output signal.