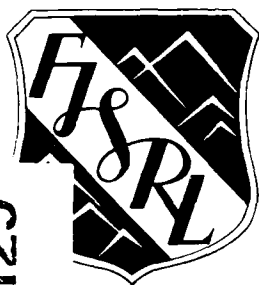


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FRANK J. SEILER RESEARCH LABORATORY

**NS(B) SPECTRUM
THEORY AND CODE**

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CAPT R.I. LAWCONNELL

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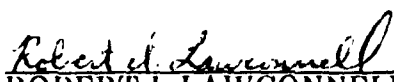
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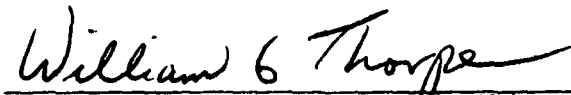
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As part of an on-going effort to determine the rotational and vibrational population of the NS(B) molecule in an $S+N_2 \rightarrow NS(B) + N_2(X)$ reaction a spectrum code was written. This document outlines the basic theory used in writing the code, explains how to run the code along with providing a listing of the spectrum code and accompanying files. It should be noted that even though this code was written specifically for the $NS(B^2\Pi) - NS(X^2\Pi)$ transition, it is easily modified to do a variety of other molecules and transitions.						
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I. INTRODUCTION

During the past year the Laser Kinetics Branch has been studying the $B^2\Pi - X^2\Pi$ transition in nitrogen-sulfide. We have been particularly interested in this transition because we think the B states 1μ second lifetime and large Franck-Condon shift make it a good short wavelength chemical laser candidate. As part of our study we have determined the rotational and vibrational populations of the excited molecule produced in an $S+N_3 \rightarrow NS(B) + N_2$ reaction. To do this accurately it was necessary to write a spectrum code. This document outlines the theory, explains how to run, and provides a listing of the spectrum code and accompanying files. It should be noted that even though this code was written specifically for the $NS(B^2\Pi) - NS(X^2\Pi)$ transition, it is easily modified to do a variety of other molecules and transitions.

II. NS SPECTRUM CODE THEORY

The code is based on the quantum mechanics of Schrödinger. In the next few pages, I'll outline the most significant relations leading up to the electronic-ro-vibrational intensity relation which gives the intensity of a spectrum line as a function of wavelength.

The perturbed Schrödinger equation is given by.

$$\sum_k \frac{1}{m_k} \left[\frac{\partial^2 \chi}{\partial X_k^2} + \frac{\partial^2 \chi}{\partial Y_k^2} + \frac{\partial^2 \chi}{\partial Z_k^2} \right] + \frac{8\pi^2}{h^2} (E-V)\chi + \omega\chi = 0 \quad (2.1)$$

where m_k is the mass of the k^{th} particle, χ is the wave function; X_k , Y_k , Z_k are the coordinates of the k^{th} particle, E is the total energy, V is the potential energy, and $\omega\chi$ is the perturbing term. The interaction of an electromagnetic wave (with an electric vector $\vec{E}$) with an atomic system can be approximated as the interaction of $\vec{E}$ with the dipole moment ($\vec{M}$) of the atomic system. This interaction enters into Equation 2.1 as $\omega = \vec{E} \cdot \vec{M}$, where $\vec{M}$ has components $M_x = \sum e_k X_k$, $M_y = \sum e_k Y_k$, $M_z = \sum e_k Z_k$, and e_k is the charge on the k^{th} particle.

In solving the Schrödinger equation for an electromagnetically disturbed atomic system, Pauling and Wilson¹ found that if the system was originally in a state of energy,

E_n , there is a non-zero probability of finding it in a state of energy, E_m , if the emission of a photon of energy $hc\nu_{nm} = E_n - E_m$ is allowed. Specifically, the probability of a transition between two states n and m is proportional to the square of the matrix elements of the electric dipole moment ($\vec{R}^{nm}$).

The components of $\vec{R}^{nm}$ are defined as follows:

$$R_x^{nm} = \int \chi_n^* M_x \chi_m d\tau, \quad (2.2)$$

$$R_y^{nm} = \int \chi_n^* M_y \chi_m d\tau, \quad (2.3)$$

$$R_z^{nm} = \int \chi_n^* M_z \chi_m d\tau, \quad (2.4)$$

where χ_n , χ_m are the eigenfunctions of the two states, and the integral is over the total configuration space.²

The intensity of a spectral line for a transition from state χ_n to χ_m is given by:

$$I_{em}^{nm} \approx N_n hc\nu_{nm} A_{nm}, \quad (2.5)$$

where N_n is the number of atoms or molecules in the initial state, $hc\nu_{nm} = E_n - E_m$ = energy emitted in transition, A_{nm} is the Einstein transition probability of spontaneous emission and according to wave mechanics is related to the matrix elements of the electric dipole moment (as was previously shown for stimulated emission) as follows:

$$A_{nm} = \frac{64\pi^4 \nu_{nm}^3}{3h} |\vec{R}^{nm}|^2 \text{ for non-degenerate levels.}$$

$$A_{nm} = \frac{64\pi^4 \nu_{nm}^3}{3h} \frac{\sum |\vec{R}^{n_i m_k}|^2}{d_p} \text{ for levels that are } d_p \text{ fold degenerate.} \quad (2.6)$$

Combining Equations (2.5) and (2.6) gives the intensity of the spectrum line in emission as:

$$I_{em}^{nm} = \frac{64\pi^4 hc\nu_{nm}^4}{3h} \frac{\sum |\vec{R}^{n_i m_k}|^2}{d_p} \quad (2.7)$$

However, our experimental detectors only count the number of photons in a given frequency range. The number of counts at a given frequency can be obtained by dividing

Equation (2.7) by the energy associated with each photon at that frequency. Doing this yields the photon count as a function of frequency:

$$I_{emc}^{nm} = \frac{64\pi^4}{3h} N_n \nu_{nm}^3 \frac{\sum |\dot{R}_{nmk}|^2}{d_p} \quad (2.8)$$

The number of molecules, N_n , in the initial state depend on the electronic, vibrational, and rotational levels available, as well as the energy required to populate each level. In the following, we will determine the energy required to populate a given electronic-rotational-vibrational state as well as the levels available. For equilibrium systems we know these states to be populated according to a Boltzmann distribution. This gives the number of molecules in each state once we know the total energy available to the system.

II.1. DETERMINATION OF ENERGY LEVELS

We know that the energy of a molecule is due to the motion of the electrons about the nuclei (electronic energy), vibration of the nuclei (vibrational energy), and rotation of the nuclei about the center of mass (rotational energy). We first will consider the rotational energy. If we approximate the molecule as a rigid rotator and substitute $m = \mu = \frac{M_1 M_2}{M_1 + M_2}$ and $V = 0$ into the Schrödinger equation (Equation 2.1), we obtain a solution for the rotational energy levels:

$$E_J = \frac{h^2 J(J+1)}{8\pi^2 I}, \quad (2.9)$$

where M_1, M_2 are the nuclear masses, and I is the moment of inertia of the rotator; J refers to the rotational level in question.

Now in spectroscopy it is customary and convenient to write all energies in terms of wave numbers. The wave number is obtained by dividing the energy by hc . So, in wave numbers Equation (2.9) becomes

$$\frac{E_J}{hc} = F(J) = \frac{hJ(J+1)}{8\pi^2 c I} = B J(J+1) \text{ (cm}^{-1}\text{)} \quad (2.10)$$

$B = \frac{h}{8\pi^2 c I}$ is called the rotational constant. The wave number (or energy) associated with a transition from one rotational level to another is:

$$\nu = F(J') - F(J''), \quad (2.11)$$

where J' always refers to the upper rotational level and J'' refers to the lower.

It is well known that molecules not only rotate about their center of mass, the nuclei vibrate with respect to one another. For a diatomic molecule, the molecule vibrates along an imaginary line joining them and passing through their respective centers. The coulombic force holding the nuclei together goes as $-kx$. The potential energy associated with this is $V = \frac{kx^2}{2}$ or that of a harmonic oscillator. If one substitutes this into the Schrödinger equation and solves for the energies of the vibrational levels, the following wave numbers (or energies) are obtained:

$$\frac{E(v)}{hc} = G(v) = \omega \left(v + \frac{1}{2} \right), \quad (2.12)$$

where ω refers to the fundamental frequency of vibration between the nuclei, and v corresponds to the allowed vibrational levels. The wave number associated with a transition from one vibrational level to another is:

$$\nu = G(v') - G(v''), \quad (2.13)$$

where v' refers to the upper vibrational level and v'' refers to the lower level.

Of course the sum of potential energy of the nuclei and the electronic energy of the electrons forms the potential well in which the nuclei carry out their vibrations. It turns out that this potential well is harmonic to first order (very small amplitude vibrations about the equilibrium displacement between the nuclei) but is anharmonic if larger displacements from equilibrium are considered. This anharmonic effect can be taken into account by using a potential of the form (instead of $V = \frac{kx^2}{2}$):

$$V = \frac{kx^2}{2} - gx^3, \quad (2.14)$$

where $x = r - r_e$, r_e is the equilibrium separation of the nuclei, and g is much smaller than $k/2$. If this potential is substituted into the Schrödinger equation, the following anharmonic-oscillator wave numbers (energies) are obtained:

$$\frac{E_v}{hc} = G(v) = \omega_e \left(v + \frac{1}{2} \right) - \omega_e x_e \left(v + \frac{1}{2} \right)^2 + \omega_e y_e \left(v + \frac{1}{2} \right)^3 + \dots \quad (2.15)$$

Previously, we considered the rotational energies of a molecule on the basis of it being a rigid rotator. It is quite obvious that if the molecule is vibrating it is not rigid. In a rather involved wave mechanical calculation, Pauling and Wilson¹ show that if one takes into account the molecular vibrations or rotations the following wave numbers for a given rotational (J) and vibrational (v) level are given:

$$F_v(J) = B_v J(J+1) - D_v J^2(J+1)^2 \quad (2.16)$$

$$\text{where } B_v = B_e - \alpha_e(v+1/2), \quad (2.17)$$

$$D_v = D_e + \beta_e(v+1/2), \quad (2.18)$$

$$B_e = \frac{h}{8\pi^2 c I_e} \quad (\text{see Equation 2.10}), \quad (2.19)$$

$$D_e = \frac{4B_e^3}{\omega_e^2}, \quad (2.20)$$

α_e and β_e are much smaller than B_e and D_e respectively.

Finally, we consider the electronic energy states associated with the electrons about the nuclei. This energy is obtained by considering the electrons interacting with each other and the nuclei. There is no exact solution of the Schödinger equation for these. One can estimate the energies of each level for a given molecule using the Born–Oppenheimer approximation.³ However, in practice the electronic energies are observed spectroscopically and used to give the base energy of each electronic level. In terms of wave numbers this energy is given by:

$$T_e = T_0 + A\Lambda\Sigma, \quad (2.21)$$

where T_0 represents the energy of the electronic state (base energy) neglecting energy splitting of levels due to electron spin, A is the spin orbit coupling constant, Λ represents the component of electronic orbital angular momentum along the internuclear axis, and Σ is the sum of electron spins for the molecule.

If the electronic orbital angular momentum is given by a vector $\vec{L}$ with magnitude $L=|\vec{L}|$ then the allowed quantum numbers representing the component of electronic angular momentum along the internuclear axis are given by:

$$\Lambda = 0, 1, 2, \dots, L \quad (2.22)$$

One should note that $\Lambda = 0, 1, 2, \dots$ corresponds to the molecular state designation $\Sigma, \Pi, \Delta, \dots$ (e.g., $\text{NS}(\text{B}^2\Pi)$ refers to nitrogen sulfide in a state with $\Lambda = 1$). T_0 in equation (2.21) above is also a function of Λ .

If the total electron spin associated with the molecule is $\vec{S}$ and the magnitude of, this spin is given by $S = |\vec{S}|$, then $\vec{S}$ will precess about the field direction (in this case the internuclear axis) with a constant component $\Sigma(\hbar/2\pi)$. Quantum theory allows the following values of $\Sigma = S, S-1, \dots -S$. (2.23)

The total number of Σ values for a given S from Equation (2.23) is given by:

$$M = 2S + 1, \quad (2.24)$$

where M is called the multiplicity of the state. The multiplet structure observed in electronic bands is due to the electron spin and the slightly different energy levels corresponding to the different electron spins given in Equation (2.23). The electronic energy of the multiplet is given by Equation (2.21). Note that if $\Lambda = 0$ for a Σ state, there can be no spin related splitting or multiplet structures. This is because when $\Lambda = 0$ there is zero orbital angular momentum of the electrons and therefore no axial magnetic field. Since this field causes the spin splitting there can be no splitting even if there is a non-zero multiplicity. So, a $^2\Sigma$ state has a multiplicity of $M=2$, but because $\Lambda=0$ there is no multiplet splitting.

The component of the total angular momentum of the electrons along the internuclear axis is given by:

$$\Omega = |\Lambda + \Sigma|. \quad (2.25)$$

This plus the quantum number for rotation (call it $\hat{N}$) of the nuclei gives the resultant total angular momentum $\hat{J}$. If the interaction of the electronic motion and the nuclear rotation is small, but the electronic motion is strongly coupled to the line joining the nuclei, Ω is well defined. This is typically referred to as a Hund's case a. There are a

variety of cases (see Hertzberg); however, for NS Hund's case a applies. So, combining all the energy (wave number) terms for a molecule we obtain the following sum:

$$\frac{E_{\text{tot}}}{hc} = T_e + G(V) + F(J) \quad (2.26)$$

The wave number associated with the emission of a photon or the transition from one state (n) to another (m) is given by:

$$\frac{h\nu'}{hc} = \nu_{nm} = T_e' - T_e'' + G(v') - G(v'') + F(J') - F(J'')$$

From Equations (2.15-2.20), this becomes:

$$\begin{aligned} \nu_{nm} = T_e' - T_e'' + \omega_e'(v'+1/2) - \omega_e'\chi_e'(v'+1/2)^2 - \omega_e''(v''+1/2) + \omega_e''\chi_e''(v''+1/2)^2 + \dots \\ + B_v'J(J+1) - D_v'J^2(J+1)^2 - B_v''J''(J''+1) + D_v''J'^2(J''+1)^2 + \dots \end{aligned} \quad (2.27)$$

This corresponds to the wave number of the emitted photon if the transition is allowed. Using quantum mechanics it is straightforward to show that molecular transitions from one particular state to another are generally allowed if:

$$\Delta J = J' - J'' = 0, \pm 1 \quad (2.28)$$

and for Hund's case a:

$$\Delta \Lambda = \Lambda' - \Lambda'' = 0, \pm 1 \quad (2.29)$$

$$\Delta \Sigma = \Sigma' - \Sigma'' = 0. \quad (2.30)$$

Note that $\Delta v = v' - v''$ is not restricted in any way.

So, if we apply this to the proposed NS(B²Π) - NS(X²Π) transition, we first note that since the upper and lower states are ²Π's, $\Lambda=1$ for both and $\Delta\Lambda=0$. Since $M=\text{multiplicity}=2S+1=2 \Rightarrow S=1/2$ or $\Sigma=\pm 1/2$. So, $\Omega=|\Lambda+\Sigma|=1/2, 3/2$. However, since $\Delta\Sigma=0$ in Hund's case a the possible electronic transitions are restricted to the following:

$$B^2\Pi_{1/2} - X^2\Pi_{1/2} \text{ and } B^2\Pi_{3/2} - X^2\Pi_{3/2},$$

where Ω has been written as the subscript on the Π (orbital angular momentum corresponding to $\Lambda=1$).

Keeping in mind that $\Delta J=0, \pm 1$ in Equation (2.27), one can represent the possible transitions for the NS(B²Π)-NS(X²Π) graphically (see Fig. 1). R₁, Q₁, P₁ correspond to

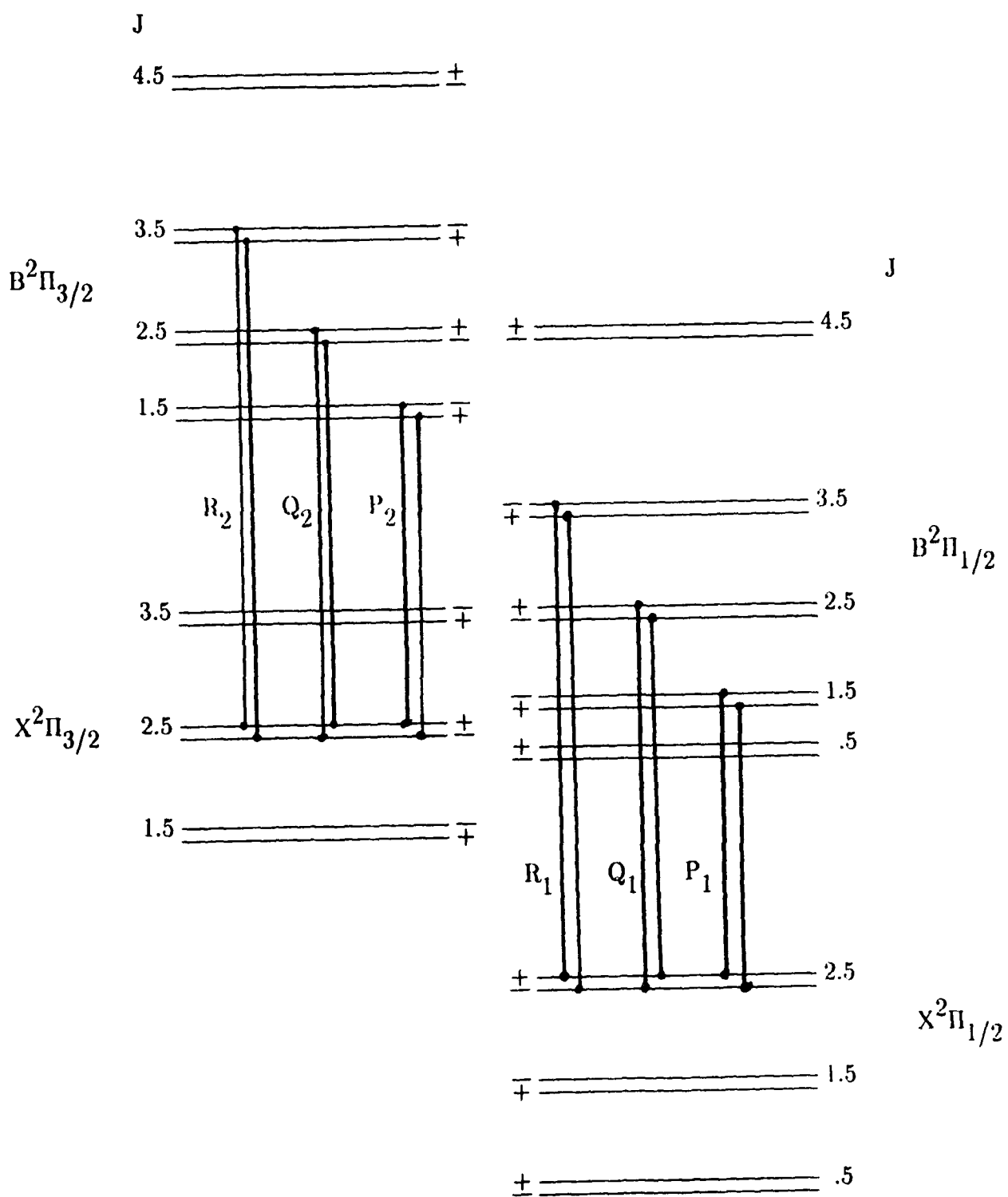


Figure 1. Energy Level Diagram for NS(B²Π)–NS(X²Π) Bands²

the branches with ΔJ s of +1, 0, -1 respectively for the $^2\Pi_{1/2}-^2\Pi_{1/2}$ transitions. R_2, Q_2, P_2 correspond to ΔJ s of +1, 0, -1 respectively for the $^2\Pi_{3/2}-^2\Pi_{3/2}$ transitions.

II.2. POPULATION OF ENERGY LEVELS

Up to this point we have considered the electronic, rotational and vibrational energy levels available to a molecule. We have also considered the allowed transitions from one state to another. Since we have determined the energy levels available we now need to figure how many molecules populate any given level. Often in nature, systems exist in states of thermal equilibrium. This is typically true of the molecules we study. For this reason we first consider obtaining the populations of electronic-rotational-vibrational energy levels for molecules in thermal equilibrium.

Electronic Distribution Function

First, we consider the electronic distribution function for a doublet state in thermal equilibrium (we consider doublets because of the doublet NS transitions). For a doublet state in equilibrium the number of molecules in the upper electronic state with a given Ω is given by (we are interested in the upper state because we want to produce an emission spectrum) a Boltzmann distribution:

$$N_{E\Omega} = \frac{N e^{-\epsilon_{\Omega}/kT_E}}{\sum_{\ell} e^{-\epsilon_{\ell}/kT_E}} \quad (2.31)$$

where ϵ_{Ω} is the energy in wave numbers of the different electronic levels associated with different values of Ω (with $\epsilon_{\min} \equiv 0$). $\min$ is the minimum Ω value and $k = .695 \text{ cm}^{-1}/^{\circ}\text{kelvin}$. For NS we have

$$N_{E1/2} = \frac{N e^{-\epsilon_{1/2}/kT_E}}{\sum_{\ell} e^{-\epsilon_{\ell}/kT_E}} = \frac{N}{e^{-\epsilon_{1/2}/kT_E} + e^{-\epsilon_{3/2}/kT_E}} \quad (2.32)$$

and with $\epsilon_{\min} = \epsilon_{1/2} = 0$, $\epsilon_{3/2} = 90$, $kT_E = 200 \text{ cm}^{-1}$ at room temperature, where $T_E = 300^{\circ}\text{K}$ = the electronic temperature.

$$N_{E_{1/2}} = N(.61)$$

$$N_{E_{3/2}} = \frac{N e^{-\epsilon_{3/2}/kT_E}}{\sum e^{-\epsilon_{\ell}/kT_E}} = N(.3893)$$

So, for NS in the B state the $\Omega=1/2$ level has 5/3 the population of the $\Omega=3/2$ level.

Vibrational Distribution Function

For vibrational levels in thermal equilibrium the population of the different energy levels is given very accurately by a Boltzmann distribution. The number of molecules in a given vibrational level is

$$N_v = \frac{N}{Q_v} e^{-G_o(v)hc/kT_v} \quad (2.33)$$

$$\text{where } Q_v = 1 + e^{-G_o(1)hc/kT_v} + \dots, \quad (2.34)$$

= state sum,

$$G_o(v) = G(v) - G(0), \quad (2.35)$$

T_v = the vibrational temperature.

It should be noted that if we are concerned with emission, $G_o(v)$ and N_v correspond to the upper state. The $G(v)$ above is given by Equation (2.15).

Rotational Distribution Function

The number of molecules found in a given rotational energy level in thermal equilibrium is given by a Boltzmann distribution function times the degeneracy of the level which is usually $2J+1$. This is because, for a given energy each of $2J+1$ degenerate levels may be populated. The number of molecules in a given J level is given by:

$$N_J = \frac{N (2J+1) e^{-F(J)hc/kT_r}}{Q_r}, \quad (2.36)$$

where $F(J)$ is given by Equation (2.16),

$$Q_r = 1 + 3e^{-F(1)hc/kT_r} + 5e^{-F(2)hc/kT_r} + \dots, \quad (2.37)$$

T_r = the rotational temperature.

Now $F(J)$, to good approximation, can often be set equal to:

$$F(J) = B_v J(J+1).$$

If this is substituted into (2.36) and (2.37),

$$Q_r = 1 + 3e^{-2B_v hc/kT_r} + 5e^{-6B_v hc/kT_r} + \dots \quad (2.38)$$

$$\approx \frac{kT_r}{hcB_v} \text{ for large } T_r \text{ and small } B_v, \text{ which is usually the case.} \quad (2.39)$$

T_r is usually greater than 300°K and B_v is about .6 for NS. This makes (2.39) a good approximation. This implies that

$$N_J \approx \frac{NhcB_v}{kT_r} (2J+1)e^{-B_v J(J+1)hc/kT_r} \quad (2.40)$$

At this point we are in a position to fairly accurately define N_n of Equation (2.8) by using (2.31), (2.33) and (2.36):

$$N_{n'} \propto N_{E\Omega'} N_{v'} N_{J'} \\ N_{n'} = \frac{N e^{-\epsilon_{\Omega'}/kT_e}}{\sum_{\ell} e^{-\epsilon_{\ell}/kT_e}} \cdot \frac{e^{-G_0(v')hc/kT_v}}{Q_{v'}} \cdot \frac{B_{v'}}{T_r} (2J'+1)e^{-B_{v'} J'(J'+1)hc/kT_r} \quad (2.41)$$

n' of course corresponds to the upper state with Ω' , J' , v' .

II.3. ELECTRONIC-RO-VIBRATIONAL INTENSITY (COUNT) FUNCTION

We almost have everything we need to define Equation (2.8) for the NS molecule. N_n of (2.8) is given by Equation (2.41), ν_{nm} of (2.8) is given by (2.27). d_p of (2.8) is equal to the degeneracy of the levels which is $2J+1$. In the literature

$$\Sigma |\hat{R}_{v'v''}^n|^2 \equiv |\hat{R}_{v'v''}|^2 S_{J'J''} \approx \hat{R}^2 q_{v'v''} S_{J'J''}, \quad (2.42)$$

where the $\hat{R}^{v'v''}$ is the part of the transition probability depending on the electronic and vibrational eigenfunctions and $S_{J'J''}$ is the part of the line strength that depends on J (the total angular momentum) and is called the Hönl-London factor.⁴ In the following we will show how $\hat{R}^{v'v''} \approx \hat{R}^2 q^{v'v''}$ and define all terms. The electronic and vibrational part of the eigenfunction can be written as:

$$\chi = \chi_e \chi_v. \quad (2.43)$$

The probability of a transition between two different (as shown in Equation (2.2-4)) electronic-vibrational states is given by:

$$|\vec{R}|^2 = |\int \chi' \vec{M} \chi d\tau|^2 \quad (2.44)$$

The only parts of the electric moment $\vec{M}$ that can contribute to $\vec{R}$ are those that depend on the coordinates of the electrons. Rewriting (2.44) and substituting (2.43) with this in mind gives:

$$\begin{aligned} \vec{R} &= \int \vec{M}_e \chi_e' \chi_e'' \chi_v' \chi_v'' d\tau \\ &= \int \chi_e' \vec{M}_e \chi_e'' d\tau_e \int \chi_v' \chi_v'' d\tau_v \end{aligned} \quad (2.45)$$

where χ_v' χ_v'' correspond to the vibrations of the nuclei along r and therefore only contribute along r , M_e and χ_e depend on the electronic coordinates only and contribute accordingly.

The first integral

$$\vec{R}_e = \int \chi_e' \vec{M}_e \chi_e'' d\tau_e, \quad (2.46)$$

is called the electronic transition moment. This transition moment depends only slightly on the internuclear separation of the nuclei. For this reason $\vec{R}_e$ is often approximated by its average value over a transition:

$$\vec{R}_e \approx \bar{\vec{R}}_e \quad (2.47)^*$$

The second integral of (2.45) is called the overlap integral. It basically states that a transition is more probable if the wave functions simultaneously have large values for the two vibrational states at a given internuclear separation. This embodies the Franck-Condon principle. As a result the overlap integral is often written in this way:

$$|\int \chi_v' \chi_v'' dr|^2 = q_{v'v''}, \quad (2.48)$$

where $q_{v'v''}$ is the Franck-Condon factor.

Note, sometimes one must include the variation $\vec{R}_e(\bar{r})$ with $\bar{r}$ to accurately model the spectrum. This happens to be the case for NS. As a function of the r -centroids ($\bar{r}_{v'v''}$) of the molecule R_e is given by:⁵

$$R_e = |\vec{R}_e(\bar{r})| = \text{Const.}(-1 + 1.767\bar{r}_{v'v''} - 1.037\bar{r}_{v'v''}^2 + .202\bar{r}_{v'v''}^3) \quad (2.49)$$

where $\bar{r}_{v'v''}$ is the average separation of the nuclei for the v' to v'' transition.

Now, all the terms are defined necessary to give the intensity of a spectral line for an electronic-ro-vibrational transition from one state to another in equilibrium. Substituting (2.41, 42) into 2.8 we have:

$$I_{J''v''\Omega}^{J'v''} = \frac{64\pi^4 N}{3h} \cdot \left[\frac{\overbrace{e^{-\epsilon_{\Omega}/kT_E}}^{N_e \text{ term}}}{\sum_{\ell} \overbrace{e^{-\epsilon_{\ell}/kT_E}}^{N_e \text{ term}}} \right] \cdot \left[\frac{\overbrace{e^{-G_o(v')hc/kT_v'}}^{N_v \text{ term}}}{Q_{v'}} \right] \cdot \left[\frac{\overbrace{B_{v'} e^{-B_{v'} J' (J'+1)hc/kT_r}}^{N_J \text{ term}}}{T_r} \right] \cdot \omega^3 \text{Re}^2 q_{v'v''} S_{J'J''} \quad (2.50)$$

For NS, we first used Equation (2.50) to obtain the equilibrium synthetic spectrum at high pressures. The synthetic spectrum closely matched the experimental spectrum.

The low pressure cases (<2 Torr) had non-equilibrium rotational and vibrational distributions. We substituted our guesses for the distributions ($N_v + N_J$ terms in (2.50) into the code until the synthetic spectrum matched the experimental spectrum. In this way we determined the non-equilibrium vibrational and rotational population distributions of the experimental spectrum. Such a comparison is shown in Figure 2, in which the relative populations of the vibrational levels $v' = 0-6$ (for $B^2\Pi_{1/2} - X^2\Pi_{1/2}$ and $B^2\Pi_{3/2} - X^2\Pi_{3/2}$ transitions) are given. The N_J term is given in FUNCTION XI of the code, run at a rotational temperature of 1400°K.

III. HOW TO RUN THE CODE

To run the NS($B^2\Pi$) – NS($X^2\Pi$) spectrum code one needs to first get in the directory where it resides. It is stored there along with files filled with Franck-Condon factors (FRANK.CON), Dunham coefficients (DUNHAM.COF), r-centroids (RCENTROID.DAT), the population weights (POPLTN.WT), file of data file names (FILE.OMA), and the experimental data files (named in FILE.OMA). These files must be present when running the program.

First one must login to the VAX as follows:

C FJ

USER: LAWCONNELL

PASSWORD: *** , see Captain Lawconnell.

Then default the directory to ASPECTRUM by typing:

Sd.ASPECTRUM

Assuming all the Dunham coefficients, Franck-Condon factors, etc., mentioned above are available, all one need do is type:

RUN SPNS

This activates the executable code found in file SPNS.EXE. The program is interactive and the input required is self-explanatory. The user will be asked to input the device on which to plot the spectrum, the spectrum title, the rotational and vibrational temperature, whether it is desired to plot experimental data versus the theory, etc. If one wishes to input non-equilibrium population weights for the upper state vibrational levels, this is done by modifying the file POPLTN.WT and specifying that a non-equilibrium distribution is required when asked while doing the input.

There is a file called INPUT.DAT that saves all the input parameters. If one is running a variety of cases that are similar this file will be accessed to give the input. The code prompts for any new changes. In addition the code produces three output files: 1) CHECK.OUT which contains the vibrational transition lines – and other information that indicates whether or not all is well with the run, 2) OUTPUT.SPEC which contains a list of intensities versus wavelength and 3) the plot file (as specified by the user).

Most features of the code are documented internally. The file structure for the various data files mentioned earlier can easily be determined by examining the respective read statements in the code. This also applies to the output files.

If one needs to transfer data from the OMA to the VAX one way to do it is to take a floppy of the data (DOS format) and use a PC along with KERMIT to transfer the data. The procedure for this is outlined below:

Type:

ZS

KERMIT

SERVER

Hit the <ALT> key

Type:

K

S (to send)

A:*. *

*. *

F (to finish)

If the procedure failed start over by typing:

<ALT>

EXIT

VAX

EXIT

and then start with the KERMIT command and proceed as before.

Finally, if one needs to modify the code to do some problem of interest it is necessary to know how the previously presented equations relate to the code. If we start at the top, the first routine encountered is the program driver. In it are documented all the references used in writing the code and for producing the input files. The program driver is responsible for the program flow from plot driver initialization, through the spectrum generation, to the output of the spectrum.

The next routine is called SUBROUTINE INPUT. It reads in the experimentally derived Dunham coefficients. Dunham's equation combines Equations (2.15-21) into one equation:

$$T = \sum_{\ell j} Y_{\ell j} (v+1/2)^j J^j (J+1)^j \quad (2.51)$$

where the $Y_{\ell j}$ are the Dunham coefficients. From Equation (2.15-21) it is easily determined that the Dunham coefficients correspond to:

$$\left[\begin{array}{cc} Y_{00} = T_e & Y_{01} = B_e \\ Y_{10} = \omega_e & Y_{11} = -\alpha_e \\ Y_{20} = -\omega_e x_e & \dots \end{array} \right] \quad \begin{array}{l} Y_{02} = -D_e \quad \dots \\ \dots \\ \dots \end{array}$$

These are the values found in the file DUNHAM.COF. We typically only use the values in the dashed box to model the NS spectra to the resolution of our spectrometer. It should be noted that there is a different group of Dunham coefficients for each electronic level - four groups for NS. This is referenced⁶ and explained in greater detail within the code.

The Franck-Condon factors ($q_v'v''$) of Equations (2.48) and (2.50) are given in file FRANK.CON.⁵ These are read in SUBROUTINE INPUT. In addition the $\bar{r}$ -centroids⁵ ($\bar{r}_v'v''$) of Equation (2.49) are also read.

If a non-equilibrium vibrational distribution is needed the N_v term of Equation (2.50) is replaced by the population weights found in file POPLN.WT. These are also read in INPUT. In addition the rotational temperature (T_r) and vibrational temperature (if equilibrium) are read in for the N_J and N_v terms of (2.50) respectively.

$G_0(v)$, Q_v , B_v , T_E , ϵ_Ω (Equations 2.15, 35; 2.34; 2.17; 2.32; 2.32 respectively) are obtained in SUBROUTINE INTENSE. These values are used there to calculate the N_E , N_v and N_J terms of Equation (2.50). All but the rotational part of Equation (2.27) is calculated in this routine and stored in matrix TRW.

The rotational part of (2.27), taking into account the P, Q, and R branching, is done in SUBROUTINE DOUBLET. This allows for the determination of the ν in equation (2.50). DOUBLET then calls SUBROUTINE AINT which gives the Hönl-London factors ($S_{J'J''}$) of equation (2.50).

Since the final intensity is normalized, the actual value of N and the constants of equation (2.50) are not important. All the terms mentioned in (2.50) are brought together in FUNCTION XI. This is where the intensity of a given spectral line is calculated. These intensities are redistributed according to a Lorentzian slit width broadening redistribution function in SUBROUTINE LORNTZN:

$$I \equiv I_0 \frac{\gamma^2}{(\lambda - 1 \times 10^8/\nu_{J'J''})^2 + \gamma^2}, \quad (2.52)$$

where γ = the spectral resolution in Angstroms (which is on the order of two Angstroms for our OMA so that Doppler broadening was not considered),

λ = the wavelength,

$1 \times 10^8/\nu_{J'J''} = \lambda_{J'J''}$ = the wavelength of the given transition one is redistributing,

I_0 = original intensity of the line.

The experimental data is read in, spliced and weighted in SUBROUTINES LOADFIL, SPLICE and WEIGHT, respectively. The data and the synthetic spectra are normalized and plotted in SUBROUTINE OUTPUT (as specified by the user).

IV. NS(B - X) SPECTRUM CODE LISTING, FILES AND SAMPLE SPECTRUM

What has been written above is embodied and takes a functional form in the following program listing. In addition, the files used to run the code are also included (they follow the code). Finally, a sample spectrum (Fig. 2) comparing the code output to experiment is included. It should be noted that the theory and experiment correspond fairly well. This was true of all the spectra generated with the code and compared to experiment (for a variety of rotational temperatures and pressures).

C PROGRAM SPECTRF

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THIS PROGRAM COMPUTES AND PLOTS THE NS(E) TO NS(X) SPECTRUM

- REFERENCES: 1) G. HERZBERG, SPECTRA OF DIATOMIC MOLECULES, VNR C 195C, P.201,268-271.
- RELATION GIVING INTENSITY OF LINE FOR TRANSITION
2) M. BORN AND R. OPPENHEIMER, ANN PHYSIK 84,457(1927).
- BORN-OPPENHEIMER APPROXIMATION
3) OBASE, ET AL, J CHEM PHYS 89,257(1988).
- FRANK-CONDON FACTORS, R CENTRICIDS, ETC. FOR NS
4) J. JEFFRIES, ET AL, J PHYS CHEM, IN PRESS, 1 DEC 87
- EXPERIMENTALLY MEASURED TRANSITION PROBABILITIES (IE. RE**2).
5) R. ENGLEMAN JR., ET AL, LA-4364, UC-34, TID-4500.
- AINT SUBROUTINE FOR NONL-CONDON FACTORS IN DOULET TO DOULET TRANSITIONS
6) I. KIVACS, ROTATIONAL STRUCTURE IN THE SPECTRA OF DIATOMIC MOLECULES, AMER. ELSEVIER PUE, CLT OF PRINT, 1969.
- BASIS OF AINT SUBROUTINE
7) K. P. HUEER AND G. HERZBERG, MOLECULAR SPECTRA AND MOLECULAR STRUCTURE, VOL IV, VNR C 1979, P486-487.
- DUNHAM COEFFICIENTS FOR NS

PARAMETER(NROT=125)

C THE COMMONS ARE DIMENSIONED AS FOLLOWS (THEY MUST BE
C DIMENSIONED GREATER THAN OR EQUAL TO THE INDICATED
C VARIABLES):

```
COMMON/FACT/F(NF,20,20),Y(ND,ND1,2),G(ND,20),
1 B(ND,20),DG(ND,20)
COMMON/P /TR(6,20,20),F1(6,NROT),P2(6,NROT),
1 F1INT(6,NROT),P2INT(6,NROT)
COMMON/Q /Q1(6,NROT),Q2(6,NROT),
1 Q1INT(6,NROT),Q2INT(6,NROT)
COMMON/R /R1(6,NROT),R2(6,NROT),R1INT(6,NROT),
1 R2INT(6,NROT),FINT(6,1000),FIN(1000),FINX(1000)
COMMON/TEMP/TV,TR
```

C WHERE, NF=NT=THE NUMBER OF GROUPS OF FRANK-CONDON FACTORS --
C 1 GROUP PER ELECTRONIC TRANSITION, I.E. B3/2 TO X3/2
C AND B1/2 TO X1/2 FOR NS.
C NF1= V PRIME MAX INDEX (UPPER STATE)
C NF2= V DOUBLE PRIME MAX INDEX (LOWER STATE)
C ND= NUMBER OF DUNHAM COEFFICIENT GROUPS --
C ONE FOR EACH OMEGA QUANTUM NUMBER

```

C      ND1= THE MAX L VALUE FOR THE DUNHAM COEFFICIENT MATRIX:
C      Y(L,J)
C      LWAV= MINIMUM WAVELENGTH OF SPECTRM (ANGSTROMS)
C      LWAV1= MAXIMUM WAVELENGTH OF SPECTRUM (ANGSTROMS)
C      NROT= NUMBER OF POSSIBLE ROTATIONAL LEVELS
C      NOTE: ALL INTEGERS USED TO DEFINE ARRAYS REFERRING TO
C      VIBRATIONAL LEVELS ARE ONE LARGER THAN THE
C      CORRESPONDING VIB. LEVEL.
C
C      CHARACTER*45  NAMDEV
C
C      CALL ASSIGN(3,'CHECK.OUT')
C      WRITE(6,*) 'WHAT TYPE OF DEVICE DO YOU WANT TO PLOT ON?'
C      WRITE(6,*) 'SPECIFY:      1      FOR HP 755C'
C      WRITE(6,*) '                2      FOR TEKTRONIX 4107'
C      WRITE(6,*) '                3      FOR VT240'
C      WRITE(6,*) '                4      FOR VT 10C RETRO'
C      WRITE(6,*) '                5      FOR TEKTRONIX 401C'
C      WRITE(6,*) '                6      FOR ANY ASCII PRINTER'
C      READ(6,*) IPLCT
C      IF(IPLCT.EQ.1) NAMDEV='HP 7550'
C      IF(IPLCT.EQ.2) NAMDEV='TEKTRONIX 4107'
C      IF(IPLCT.EQ.3) NAMDEV='VT 240'
C      IF(IPLCT.EQ.4) NAMDEV='VT 10C RETRO'
C      IF(IPLCT.EQ.5) NAMDEV='TEKTRONIX 4010'
C      IF(IPLCT.EQ.6) NAMDEV='ANY ASCII PRINTER'
C      CALL PLTDEV(NAMDEV)
C      CALL INPUT
C      CALL INTENSE
C      CALL OUTPUT
C      CALL DCNEPL
C      CALL CLOSE(3)
C      STOP
C      END
C      SUBROUTINE INPUT
C      PARAMETER(NROT=125)
C      COMMON/FACT/F(3,30,30),Y(9,30,2),G(9,30),
C      1 B(9,30),DG(9,30)
C      COMMON/P /TR(6,30,30),P1(6,NROT),P2(6,NROT),
C      1 P1INT(6,NROT),P2INT(6,NROT)
C      COMMON/G /Q1(6,NROT),Q2(6,NROT),
C      1 Q1INT(6,NROT),Q2INT(6,NROT)
C      COMMON/R /R1(6,NROT),R2(6,NROT),R1INT(6,NROT),
C      1 R2INT(6,NROT),FINT(6,1000),FIN(1000),FINX(1000)
C      COMMON/TEMP/TV,TR
C      COMMON/INPLT/NTITLE,IFDIS,IBRANCH,WPIN,WMAX,RRES,
C      1 XTV,XTR,IFDONE,IFDEF,IPIN,IPAX,IENVH,EAVH1,V,
C      2 XP,TK,GAMPA2
C      COMMON/INDEX/NF,NF1,NF2,NT,ND,AD1
C      COMMON/WGHT/WGHT(30,30),NVIB,IFEXCIT
C      COMMON/CNTR/CNTR(3,30,30),IFCENTR
C      COMMON/EXPDAT/IFDATA,WAVE(20,1030),SPEC(20,1030),WAV(20000),
C      1 SP(20000),WW(20000),SPW(20000),WDAT(20),SEA(20),ICCUNT,IIPAX,
C      2 IAMAX,BKGFND,SLOPE
C      COMMON/PERT/IFPERT,TRP,IFPLB,VAR,VAR1,VAR2
C      CHARACTER*40  ATITLE
C      CHARACTER*30  IFILE
C
C      READ IN THE APPROPRIATE FRANK CONDENSED FACTORS

```

```

C
  CALL ASSIGN(2,'FRANK.CON')
  READ(2,*) NF,NF1,NF2,NT
  WRITE(3,*) NF,NF1,NF2,NT
  DO 10 N=1,NF
C N=1 IMPLIES B1/2 -- X1/2 ELECTRONIC TRANSITION
C N=2 IMPLIES B3/2 -- X3/2 ELECTRONIC TRANSITION
    DO 20 I=1,NF1
      READ(2,*) (F(N,I,IP),IP=1,NF2)
      WRITE(3,*) (F(N,I,IP),IP=1,NF2)
    20 CONTINUE
    10 CONTINUE
    CLCSE(2)
C
C READ IN THE DUNHAM COEFFICIENTS
C
C NOTE: THE ZERO POINT ENERGIES ARE INCLUDED IN THE FIRST
C DUNHAM COEFFICIENT IN THIS FORMULATION
C
  CALL ASSIGN(2,'DUNHAM.CCF')
  READ(2,*) ND,ND1
  WRITE(3,*) ND,ND1
  DO 30 M=1,ND
C M=1 IMPLIES X2F11/2 STATE
C M=2 IMPLIES B2F11/2 STATE
C M=3 IMPLIES X2F13/2 STATE
C M=4 IMPLIES B2F13/2 STATE
    DO 40 L=1,ND1
      READ(2,*) Y(M,L,1),Y(M,L,2)
    40 CONTINUE
    DO 39 L=1,ND1
      WRITE(3,*) Y(M,L,1),Y(M,L,2)
    39 CONTINUE
    30 CONTINUE
    CALL CLCSE(2)
    WRITE(6,*) 'IF YOU HAVE NOT DONE THIS SPECTRUM BEFORE OR WOULD',
1 ' LIKE TO START FROM SCRATCH TYPE: C , OTHERWISE TYPE: 1 .'
    READ(6,*) IFDONE
    IF(IFDONE.EQ.0) THEN
      WRITE(6,*) 'WHAT DO YOU WANT TO ENTITLE YOUR SPECTRUM?'
      READ(6,33) NTITLE
    33 FORMAT(A30)
      WRITE(6,*) 'IF YOU WANT THE CODE TO DETERMINE THE MINIMUM AND',
2 ' MAXIMUM WAVELENGTHS BETWEEN WHICH THE SPECTRUM IS TO BE',
3 ' PLOTTED TYPE: C ',
4 ' NOTE: THIS RESOLVES THE SPECTRUM ON 2000 POINTS IN WAVELENGTH'
      READ(6,*) IFDEF
      IF(IFDEF.NE.C) THEN
        WRITE(6,*) 'WHAT IS THE MINIMUM WAVELENGTH(WPIN) IN ANGSTROM?'
        READ(6,*) WPIN
        WRITE(6,*) 'WHAT IS THE MAXIMUM WAVELENGTH(WPAX) IN ANGSTROM?'
        READ(6,*) WPAX
        WRITE(6,*) 'WHAT RESOLUTION(RES) DO YOU DESIRE IN THE SPECTRUM?'
        WRITE(6,*) 'NOTE:(WPAX-WPIN)/RES .LE. 10000 AND MUST BE AN',
1 ' INTEGER'
        READ(6,*) RRES
      ENDIF
      WRITE(6,*) 'WHAT IS THE VIBRATIONAL TEMPERATURE (DEG KELVIN)?'
      READ(6,*) XTV
      WRITE(6,*) 'WHAT IS THE ROTATIONAL TEMPERATURE (DEG KELVIN)?'

```

```

READ(6,*) XTR
WRITE(6,*) 'DO YOU WANT A LORENTZIAN (C) OR GAUSSIAN (1)?',
1 'DISTRIBUTION (GAUSSIAN NOT YET IMPLEMENTED)?'
READ(6,*) IFDIS
IF(IFDIS.EQ.0) THEN
  WRITE(6,*) 'WHAT IS GAMMA**2 FOR LORENTZIAN? IF C IS RETURNED',
1 'GAMMA**2=9.5E'
  READ(6,*) GAMPA2
  IF(GAMPA2.EQ.C) THEN
    GAMPA2=9.58
  ENDIF
ENDIF
IF(IFDIS.EQ.1) THEN
  WRITE(6,*) 'WHAT IS THE GAS KINETIC TEMPERATURE (KELVIN)?'
  READ(6,*) TK
  WRITE(6,*) 'WHAT IS THE EMITTING MOLECULES MOLECULAR WEIGHT',
1 '(GRAMS/MOLE)?'
  READ(6,*) XM
ENDIF
WRITE(6,*) 'WHAT IS THE EXPECTED ENVELOPE WIDTH OF THE',
1 'THE DISTRIBUTION (IN ANGSTROMS)-- IF ZERO IS RETURNED THE',
2 'CODE WILL ESTIMATE A VALUE.'
READ(6,*) ENVH1
WRITE(6,*) 'WHAT TYPE OF ROTATIONAL BRANCHING IS REQUIRED?'
WRITE(6,*) 'THE CHOICES ARE: '
WRITE(6,*) '1) P1,Q1,R1,F2,Q2,R2 FOR 2PI--2PI TRANSITIONS'
WRITE(6,*) 'CORRESPONDING TO HLNDS CASE A.'
READ(6,*) IBRANCH
WRITE(6,*) 'IF YOUR UPPER ELECTRONIC STATE HAS A NON-EQUILIBRIUM'
WRITE(6,*) 'VIBRATIONAL DISTRIBUTION TYPE: 1 '
WRITE(6,*) 'OTHERWISE TYPE: C '
WRITE(6,*) 'HAVE THE RELATIVE WEIGHTS OF EACH VIBRATIONAL LEVEL'
WRITE(6,*) 'IN FILE POPLTN.WT'
READ(6,*) IFEXCIT
IF(IFEXCIT.EQ.1) THEN
  CALL ASSIGN(2,'POPLTN.WT')
  READ(2,*) NVIB
C NVIB IS THE NUMBER OF VIBRATIONAL LEVELS IN THE UPPER STATE YOU HAVE
C WEIGHTS FOR. ALSO THERE IS ONE SET OF WEIGHTS FOR EACH TRANSITION.
  DO 50 N=1,NF
    READ(2,*) (WGHT(N,I),I=1,NVIB)
    WRITE(3,*) (WGHT(N,I),I=1,NVIB)
50  CONTINUE
  CALL CLOSE(2)
ENDIF
WRITE(6,*) 'IF YOU WANT TO WEIGHT THE SPECTRAL INTENSITIES'
WRITE(6,*) 'WITH THE R-CENTROIDS TYPE: 1 '
WRITE(6,*) 'OTHERWISE TYPE: 0'
WRITE(6,*) 'THE R-CENTROIDS ARE ASSUMED TO BE IN RCENTROID.DAT'
READ(6,*) IFCENTR
IF(IFCENTR.EQ.1) THEN
  CALL ASSIGN(2,'RCENTROID.DAT')
  DO 70 N=1,NF
C N=1 IMPLIES B1/2 -- X1/2 ELECTRONIC TRANSITION
C N=2 IMPLIES B3/2 -- X3/2 ELECTRONIC TRANSITION
C THERE SHOULD BE AS MANY R-CENTROIDS AS FRANK-CONDON FACTORS
    DO 80 I=1,NF1
      READ(2,*) (CNTR(N,I,IP),IP=1,NF2)
      WRITE(3,*) (CNTR(N,I,IP),IP=1,NF2)
80  CONTINUE

```

```

70  CONTINUE
    CALL CLOSE(2)
    ENDIF
WRITE(6,*) 'INCLUDE NON-BOLTZMANN CONTRIBUTION TO ROTATIONAL'
WRITE(6,*) 'LEVELS AS SPECIFIED BELOW ? YES (1), NO (0). '
READ(6,*) IFPERT
IF(IFPERT.EQ.1) THEN
    WRITE(6,*) 'WHAT IS THE PSEUDO ROTATIONAL TEMPERATURE (K)? '
    READ(6,*) TRF
    WRITE(6,*) 'WHAT IS THE RELAT HEIGHT OF 2ND EXP FOR ROT DIS? '
    READ(6,*) VAR
    WRITE(6,*) 'AT WHICH ROT. LINE DOES COUNT. TAKE EFFECT '
    READ(6,*) VAR1
    VAR2=VAR1-1
ENDIF
WRITE(6,*) 'PUBLICATION QUALITY (GRAPHS BLACK)? YES (1), NO (0). '
READ(6,*) IFPUE
WRITE(6,*) 'DO YOU WANT TO PLOT THE THEORETICAL AND EXPERIMENTAL '
WRITE(6,*) 'SPECTRA ON THE SAME GRAPH? YES (1) , NO (0) '
READ(6,*) IFDATA
IF(IFDATA.EQ.1) THEN
    WRITE(6,*) 'SPECIFY THE THE AVERAGE NUMBER OF BACKGROUND COUNTS '
    WRITE(6,*) 'PER PIXEL TO SUBTRACT FROM YOUR DATA. DO THIS BY '
    WRITE(6,*) 'FIRST SPECIFYING THE INITIAL NUMBER OF COUNTS TO '
    WRITE(6,*) 'SUBTRACT AT YOUR MINIMUM WAVELENGTH '
    READ(6,*) EKGRND
    WRITE(6,*) 'NOW SPECIFY THE SLOPE OF THE LINE OF THE '
    WRITE(6,*) 'AVERAGE INCREASE IN COUNTS/ANGSTROM '
    READ(6,*) SLOPE
    WRITE(6,*) 'YOUR SPECTRAL DATA IS ASSUMED TO BE IN THE '
    WRITE(6,*) 'FILES NAMED IN : FILE.CMA. NOTE THAT IT IS '
    WRITE(6,*) 'ALSO ASSUMED THAT THE FIRST FILE LISTED IN FILE.OMA '
    WRITE(6,*) 'CORRESPONDS TO THE LOWEST WAVELENGTH AND SO ON '
    WRITE(6,*) 'IT IS ALSO ASSUMED THERE ARE NO GAPS IN WAVELENGTH '
    WRITE(6,*) 'BETWEEN CONSECUTIVE OMA FILES. '
ENDIF
IF(IFDATA.NE.1) THEN
    WRITE(6,*) 'CALCULATING THE SYNTHETIC SPECTRA... '
    WRITE(6,*) 'CRUNCH...CRUNCH...CRUNCH... '
ENDIF
ELSE
    WRITE(6,*) 'WHAT IS THE NAME OF YOUR INPUT FILE (TYPICALLY ',
1  ' INPLT.DAT)? '
    READ(6,35) IFILE
    CALL ASSIGN(2,IFILE)
    READ(2,*) WMIN,WMAX,RRES,XIV,XTR
    READ(2,35) NTITLE
35  FORMAT(A30)
36  FORMAT(1X,A30)
    READ(2,*) IFDIS,IERANCH,ENVH1,TK,XP,GAMMA2
    READ(2,*) IFXCIT,IFCENTR
    CALL CLOSE(2)
    WRITE(6,*) 'THE INPUT.DAT FILE HAS THE FOLLOWING VARIABLE',
1  ' VALUES: '
    WRITE(6,*) 'THE PLOT TITLE IS 1: '
    WRITE(6,36) NTITLE
    WRITE(6,*) 'LORENTZIAN(0) OR GAUSSIAN(1) DIS. 2: ',IFDIS
    WRITE(6,*) 'THE ENVELOPE HALF WIDTH OF DIS. 3: ',ENVH1
    WRITE(6,*) 'THE BRANCHING IS GIVEN BY '
    WRITE(6,*) '1) 2PI--2PI,HLNDS CASE A 4: ',IERANCH

```

```

WRITE(6,*) 'THE MINIMUM WAVELENGTH(A) IS      5:',WMIN
WRITE(6,*) 'THE MAXIMUM WAVELENGTH(A) IS      6:',WMAX
IFDEF=1
WRITE(6,*) 'THE MIN RESOLUTION IN ANGSTOMS    7:',RRES
WRITE(6,*) 'THE VIBRATIONAL TEMP (KELVIN) IS  8:',XTV
WRITE(6,*) 'THE ROTATIONAL TEMP (KELVIN) IS   9:',XTR
IF(IFDIS.EQ.0) THEN
WRITE(6,*) 'GAPMA**2 IS                      10:',GAPMA2
ENDIF
IF(IFDIS.EQ.1) THEN
WRITE(6,*) 'THE GAS KINETIC TEMP (KELVIN) IS 11:',TK
WRITE(6,*) 'THE MOLECULAR WEIGHT (G/MOLE) IS 12:',XM
ENDIF
WRITE(6,*) 'THE UPPER STATE VIBRATIONAL LEVELS'
WRITE(6,*) 'ARE IN EQUILIBRIUM (0) OR THEY ARE'
WRITE(6,*) 'EXCITED (1)                      13:',IFEXCIT
WRITE(6,*) 'INCLUDE R-CENTROIDS,YES(1),NO(0) 14:',IFCENTR
WRITE(6,*) '***WHICH OF THE ABOVE VARIABLES DO YOU',
1 ' WANT TO CHANGE? TYPE 0 WHEN YOU ARE FINISHED',
2 ' MAKING CHANGES. ENTER NUMBERS ONE AT A TIME.'
DO 15C I=1,14
READ(6,*) IVAR
IF(IVAR.EQ.0) GO TO 16C
IF(IVAR.EQ.1) THEN
WRITE(6,*) 'PLOT TITLE:'
READ(6,35) NTITLE
ENDIF
IF(IVAR.EQ.2) THEN
WRITE(6,*) 'DISTRIBUTION (0 OR 1):'
READ(6,*) IFDIS
IF(IFDIS.EQ.0) THEN
WRITE(6,*) 'REMEMBER TO MODIFY VARIABLES 11 AND 12'
ENDIF
ENDIF
IF(IVAR.EQ.3) THEN
WRITE(6,*) 'ENVELOPE HALF WIDTH (ANGSTROMS):'
READ(6,*) ENVH1
ENDIF
IF(IVAR.EQ.4) THEN
WRITE(6,*) 'BRANCHING IS:'
READ(6,*) IBRANCH
ENDIF
IF(IVAR.EQ.5) THEN
WRITE(6,*) 'MIN WAVELENGTH (ANGSTROMS):'
READ(6,*) WMIN
ENDIF
IF(IVAR.EQ.6) THEN
WRITE(6,*) 'MAX WAVELENGTH (ANGSTROMS):'
READ(6,*) WMAX
ENDIF
IF(IVAR.EQ.7) THEN
WRITE(6,*) 'RESOLUTION (ANGSTROMS):'
READ(6,*) RRES
ENDIF
IF(IVAR.EQ.8) THEN
WRITE(6,*) 'VIB TEMPERATURE (KELVIN):'
READ(6,*) XTV
ENDIF
IF(IVAR.EQ.9) THEN
WRITE(6,*) 'ROT TEMPERATURE (KELVIN):'

```

```

      READ(6,*) XTR
    ENDIF
    IF(IVAR.EQ.10) THEN
      WRITE(6,*) 'GAMMA**2 IS:'
      READ(6,*) GAMMA2
    ENDIF
    IF(IVAR.EQ.11) THEN
      WRITE(6,*) 'GAS KINETIC TEMPERATURE (KELVIN):'
      READ(6,*) TK
    ENDIF
    IF(IVAR.EQ.12) THEN
      WRITE(6,*) 'MOLECULAR WEIGHT (GRAMS/MOLE):'
      READ(6,*) XM
    ENDIF
    IF(IVAR.EQ.13) THEN
      WRITE(6,*) 'UPPER STATE VIBRATIONAL EXCITATION'
      WRITE(6,*) 'EQUILIBRIUM (C), NON-EQUILIBRIUM (1):'
      READ(6,*) IFEXCIT
    ENDIF
    IF(IVAR.EQ.14) THEN
      WRITE(6,*) 'INCLUDE R-CENTRICIDS? YES(1) OF NO(C):'
      READ(6,*) IFCENTR
    ENDIF
150  CONTINUE
160  CONTINUE
      IF(IFEXCIT.EQ.1) THEN
        CALL ASSIGN(2,'PCPLTN.WT')
        READ(2,*) NVIE
C NVIE IS THE NUMBER OF VIBRATIONAL LEVELS IN THE UPPER STATE YOU HAVE
C WEIGHTS FOR. ALSO THERE IS ONE SET OF WEIGHTS FOR EACH TRANSITION.
        DO 60 N=1,NF
          READ(2,*) (WGHT(N,II),II=1,NVIB)
          WRITE(3,*) (WGHT(N,II),II=1,NVIB)
60    CONTINUE
          CALL CLOSE(2)
        ENDIF
        IF(IFCENTR.EQ.1) THEN
          CALL ASSIGN(2,'RCENTRID.DAT')
          DO 85 N=1,NF
C N=1 IMPLIES B1/2 -- X1/2 ELECTRONIC TRANSITION
C N=2 IMPLIES B3/2 -- X3/2 ELECTRONIC TRANSITION
C THERE SHOULD BE AS MANY R-CENTRICIDS AS FRANK-CONDON FACTORS
          DO 90 II=1,NF1
            READ(2,*) (CNTR(N,II,IP),IP=1,NF2)
            WRITE(3,*) (CNTR(N,II,IP),IP=1,NF2)
90    CONTINUE
85    CONTINUE
            CALL CLOSE(2)
          ENDIF
          WRITE(6,*) 'INCLUDE NON-BOLTZMANN CONTRIBUTION TO ROTATIONAL'
          WRITE(6,*) 'LEVELS AS SPECIFIED BELOW ? YES (1), NO (0). '
          READ(6,*) IFPERT
          IF(IFPERT.EQ.1) THEN
            WRITE(6,*) 'WHAT IS THE PSEUDO ROTATIONAL TEMPERATURE (K)?'
            READ(6,*) TRF
            WRITE(6,*) 'WHAT IS THE RELAT HEIGHT OF 2ND EXP FOR ROT DIS?'
            READ(6,*) VAR
            WRITE(6,*) 'AT WHICH ROT. LINE DOES CONT. TAKE EFFECT'
            READ(6,*) VAR1
            VAR2=VAR1-1

```

```

ENDIF
WRITE(6,*) 'PUBLICATION QUALITY (GRAPHS BLACK)? YES (1), NC (0).'
```

READ(6,*) IFPUE

```

WRITE(6,*) 'DO YOU WANT TO PLOT THE THEORETICAL AND EXPERIMENTAL'
WRITE(6,*) 'SPECTRA ON THE SAME GRAPH? YES (1) , NC (0)'
```

READ(6,*) IFDATA

```

IF(IFDATA.EQ.1) THEN
WRITE(6,*) 'SPECIFY THE THE AVERAGE NUMBER OF BACKGROUND COUNTS'
WRITE(6,*) 'PER PIXEL TO SUBTRACT FROM YOUR DATA. DO THIS BY'
WRITE(6,*) 'FIRST SPECIFYING THE INITIAL NUMBER OF COUNTS TO'
WRITE(6,*) 'SUBTRACT AT YOUR MINIMUM WAVELENGTH'
```

READ(6,*) EKGRND

```

WRITE(6,*) 'NOW SPECIFY THE SLOPE OF THE LINE OF THE'
WRITE(6,*) 'AVERAGE INCREASE IN COUNTS/ANGSTROM'
```

READ(6,*) SLOPE

```

WRITE(6,*) 'YOUR SPECTRAL DATA IS ASSUMED TO BE IN THE '
WRITE(6,*) 'FILES NAMED IN : FILE.CMA. NOTE THAT IT IS'
WRITE(6,*) 'ALSO ASSUMED THAT THE FIRST FILE LISTED IN FILE.OMA'
WRITE(6,*) 'CORRESPONDS TO THE LOWEST WAVELENGTH AND SO ON '
WRITE(6,*) 'IT IS ALSO ASSUMED THERE ARE NO GAPS IN WAVELENGTH'
WRITE(6,*) 'BETWEEN CONSECUTIVE OMA FILES.'
```

ENDIF

```

IF(IFDATA.NE.1)THEN
WRITE(6,*) 'CALCULATING THE SYNTHETIC SPECTRA...'
```

WRITE(6,*) 'CRUNCH...CRUNCH...CRUNCH...'

ENDIF

ENDIF

```

TV=XTV*.695
TR=XTR*.695
IF(IFDIS.EQ.1) THEN
V=SQRT(2.494E8*TK/XM)*1E8
ENDIF
RETURN
END
```

SUBROUTINE INTENSE

```

PARAMETER(NROT=125)
COMMON/FACT/F(3,30,30),Y(9,30,2),G(9,30),
1 B(9,30),DG(9,30)
COMMON/P /TRW(6,30,30),P1(6,NROT),P2(6,NROT),
1 P1INT(6,NROT),P2INT(6,NROT)
COMMON/G /Q1(6,NROT),Q2(6,NROT),
1 Q1INT(6,NROT),Q2INT(6,NROT)
COMMON/R /R1(6,NROT),R2(6,NROT),R1INT(6,NROT),
1 R2INT(6,NROT),FIN(6,1000),FIN(1000),FINX(1000)
COMMON/TEMP/TV,TR
COMMON/INPUT/NTITLE,IFDIS,IERANCH,LPMIN,LMAX,RRES,
1 XTV,XTR,IFDONE,IFDEF,IMIN,IMAX,IENVH,EAVH1,V,
2 XP,TK,GAMMA2
COMMON/INDEX/NF,NF1,NF2,NT,ND,ND1
COMMON/WGHT/WGHT(30,30),NVIB,IFEXCIT
COMMON/CNTR/CNTR(3,30,30),IFCENTR
COMMON/EXPDAT/IFDATA,WAVE(20,1030),SPEC(20,1030),WAV(2000),
1 SP(2000),LW(2000),SPW(2000),WDAT(20),SEN(20),ICCOUNT,IIMAX,
2 INMAX,BKGRND,SLOPE
COMMON/SPIN/NC
CHARACTER*4C NTITLE
```

C
C
C

CALCULATE ENERGIES (G) AND MOLECULAR CONSTANTS (E) FOR

```

C   VIBRATIONAL LEVELS
C
      NMAX=MAX(NF1,NF2)
      DO 10 M=1,ND
      DO 20 I=1,NMAX
      G(M,I)=0.
      B(M,I)=C.
      DO 30 L=1,ND1
C
      IEP=L-1
      XI=FLOAT(I)
      G(M,I)=G(M,I)+Y(M,L,1)*((XI-1.)+.5)**(IEP)
      B(M,I)=B(M,I)+Y(M,L,2)*((XI-1.)+.5)**(IEP)
C      WRITE(3,*) 'G,M,I=',G(M,I),M,I
30    CONTINUE
      WRITE(3,*) 'G,M,I=',G(M,I),M,I
C
C   CALCULATE THE ENERGY DIFFERENCE (DG) BETWEEN VIBRATIONAL
C   LEVEL I AND THE LOWEST VIBRATIONAL LEVEL WITHIN THE ELECTRONIC STAT
C
      DG(M,I)=G(M,I)-G(M,1)
      WRITE(3,*) 'DG,M,I=',DG(M,I),M,I
C
20    CONTINUE
10    CONTINUE
C
C   CALCULATE THE VIBRATIONAL LEVEL TRANSITION (TR)
C   FREQUENCIES BETWEEN THE UPPER AND LOWER ELECTRONIC
C   LEVELS -- HUNDS CASE A.
C
      NN=1
      DO 40 N=1,NF
      DO 50 I=1,NF1
      DO 60 IP=1,NF2
      TRW(N,I,IP)=G(NN+1,I)-G(NN,IP)
      WRITE(3,*) 'TRANS',TRW(N,I,IP),N,I,IP
C   NOTE: BP-BPP<C FOR RED DEGRADED BANDS
C         BP-BPP>C FOR BLUE DEGRADED BANDS
      WRITE(3,*) 'BP-BPP=',B(NN+1,I)-B(NN,IP)
60    CONTINUE
50    CONTINUE
      NN=NN+2
40    CONTINUE
C
C   DETERMINE THE MIN AND MAX EXTENT OF THE PESH IN ANGSTOMS
C   IF NOT SET IN THE INPUT
C
      IF(IFDEF.EG.0) THEN
      WMIN=1E20
      WMAX=C.
      DO 41 N=1,NF
      DO 51 I=1,NF1
      DO 61 IP=1,NF2
      XW=1.E8/TRW(N,I,IP)
      WMAX=MAX(XW,WMAX)
      WMIN=MIN(XW,WMIN)
61    CONTINUE
51    CONTINUE
41    CONTINUE
      RRES=(WMAX-WMIN)/2C00.

```



```

ENDIF
C
C IF THERE IS A NON-EQUILIBRIUM DISTRIBUTION OF
C VIBRATIONAL LEVELS THEY ARE SET HERE
C
IF(IFEXCIT.EQ.1.AND.NVIB.GE.I) EXPV=WGHT(N,I)
C
C IF ONE REQUIRES THE INCLUSION OF THE R-CENTROIDS IN THE
C COMPUTATION OF THE INTENSITIES THEIR CONTRIBUTION IS
C TAKEN INTO ACCOUNT NEXT
C
IF(IFCENTR.EQ.1) THEN
  RE=-1.+1.76711*CNTR(N,I,IP)-1.03755*CNTR(N,I,IP)**2
  +2.028*CNTR(N,I,IP)**3
  EXPV=EXPV*RE**2
ENDIF
C
C THE LAMEDA TYPE DOUPLING OF EACH MULTIPLET(TWO OF THEM NC=1,2)
C IS TAKEN INTO ACCOUNT IN THE NC LOOP. THE EFFECT OF THE FUNCTIONS
C FP AND FPP CHANGE ACCORDINGLY.
C
DO 72 NC=1,2
  IF(IERANCH.EQ.1) CALL DCUBLET(N,NN,I,IP,EXPV)
  WRITE(3,*) 'F,I,IP,EXPV=',F(N,I,IP),I,IP,EXPV
C
C REDISTRIBUTE INTENSITIES WITH LORENTZIAN -DUE TO HOMOGENEOUS SLIT
C RELATED BROADENING
C
IF(IFDIS.EQ.0) THEN
  CALL LORNTZN(N,I,IP)
72 CONTINUE
90 CONTINUE
80 CONTINUE
  NN=NN+2
75 CONTINUE
  RETURN
  END
  SUBROUTINE DOUBLET(N,NN,I,IP,EXPV)
  PARAMETER(NROT=125)
  COMMON/FACT/F(3,30,30),Y(9,30,2),G(9,30),
1 B(9,30),DG(9,30)
  COMMON/P /TR6(6,30,30),P1(6,NROT),P2(6,NROT),
1 P1INT(6,NROT),P2INT(6,NROT)
  COMMON/G /Q1(6,NROT),G2(6,NROT),
1 Q1INT(6,NROT),G2INT(6,NROT)
  COMMON/R /R1(6,NROT),R2(6,NROT),R1INT(6,NROT),
1 R2INT(6,NROT),FINT(6,1000),FIN(1000),FINX(1000)
  COMMON/TEMP/TV,TR
  COMMON/INPLT/NTITLE,IFDIS,IERANCH,LPMIN,LMAX,RRES,
1 XTV,XTR,IFDONE,IFDEF,IPIN,IMAX,IENVH,ENVH1,V,
2 XP,TK,GAMMA2
  COMMON/INDEX/NF,NF1,NF2,NT,ND,ND1
  DATA DE,DEP,AP,APP/1.2E-6,1.3E-6,149.7,285.8/
C YY AND YE ARE THE LOWER AND UPPER STATE SPIN ORBIT SPLITTING
C WAVE NUMBERS.
  DATA P,PE,YY,YE/1.,1.,221.5,90./
C
  DATA F,FE,YY,YE/1.,1.,10000,10000/
  CHARACTER*4C ATITLE
  IF(N.EQ.1) THEN
    Z=.5

```

```

ZE=.5
ELSE
Z=1.5
ZE=1.5
ENDIF
DO 100 J=1,NROT
IF(N.EG.1) THEN
C N EQ 1 MEANS WE'RE DOING BPI1/2--XPI1/2 TRANSITIONS
C P1-BRANCH
R=FLOAT(J)-.5
RE=R-1
P1(N,J)=TRW(N,I,IP)+FP(R-1,NN,I,P,YE,DE)-FPP(R,NN,IP,P,YY,DEP)
FR=P1(N,J)
C NOTE: THE COMPILER WAS HAVING A PROBLEM RECOGNIZING P1 IN THE
C XI FUNCTION CALL UNTIL I SET FR=P1(N,J) AND PASSED FR IN THE
C XI FUNCTION CALL, AS YOU SEE BELOW. BEFORE THE CHANGE, AT RUN
C TIME, FR WITHIN THE XI FUNCTION CALL WAS UNDEFINED = ZERO.
CALL AINT(SJ,P,R,Z,YY,RE,PE,ZE,YE)
P1INT(N,J)=XI(N,NN,I,IP,SJ,FR,RE,EXPV,YY)
C
WRITE(6,*) 'SJ OF P1=',SJ
C
WRITE(6,*) N,J,P1(N,J),P1INT(N,J)
C Q1-BRANCH
RE=R
Q1(N,J)=TRW(N,I,IP)+FP(R,NN,I,P,YE,DE)-FPP(R,NN,IP,P,YY,DEP)
FR=Q1(N,J)
CALL AINT(SJ,P,R,Z,YY,RE,PE,ZE,YE)
Q1INT(N,J)=XI(N,NN,I,IP,SJ,FR,RE,EXPV,YY)
C R1-BRANCH
RE=R+1.
R1(N,J)=TRW(N,I,IP)+FP(R+1,NN,I,P,YE,DE)-FPP(R,NN,IP,P,YY,DEP)
FR=R1(N,J)
CALL AINT(SJ,P,R,Z,YY,RE,PE,ZE,YE)
R1INT(N,J)=XI(N,NN,I,IP,SJ,FR,RE,EXPV,YY)
ELSE
C N EQ 2 MEANS WE'RE DOING BPI3/2--XPI3/2 TRANSITIONS
C P2-BRANCH
R=FLOAT(J)+.5
RE=R-1.
P2(N,J)=TRW(N,I,IP)+FP(R-1,NN,IP,P,YE,DE)-FPP(R,NN,IP,P,YY,DEP)
FR=P2(N,J)
CALL AINT(SJ,P,R,Z,YY,RE,PE,ZE,YE)
P2INT(N,J)=XI(N,NN,I,IP,SJ,FR,RE,EXPV,YY)
C
WRITE(6,*) 'SJ OF P2=',SJ
C
WRITE(6,*) N,J,P2(N,J),FR,P2INT(N,J)
C Q2-BRANCH
RE=R
Q2(N,J)=TRW(N,I,IP)+FP(R,NN,IP,P,YE,DE)-FPP(R,NN,IP,P,YY,DEP)
FR=Q2(N,J)
CALL AINT(SJ,P,R,Z,YY,RE,PE,ZE,YE)
Q2INT(N,J)=XI(N,NN,I,IP,SJ,FR,RE,EXPV,YY)
C R2-BRANCH
RE=R+1.
R2(N,J)=TRW(N,I,IP)+FP(R+1,NN,IP,P,YE,DE)-FPP(R,NN,IP,P,YY,DEP)
FR=R2(N,J)
CALL AINT(SJ,P,R,Z,YY,RE,PE,ZE,YE)
R2INT(N,J)=XI(N,NN,I,IP,SJ,FR,RE,EXPV,YY)
ENDIF
100 CONTINUE
RETURN
END

```

```

REAL FUNCTION FF(R,NN,I,P,YE,DE)
PARAMETER(NROT=125)
COMMON/FACT/F(3,30,30),Y(9,30,2),G(9,30),
1 B(9,30),DG(9,30)
COMMON/F /TR(6,30,30),P1(6,NROT),P2(6,NROT),
1 P1INT(6,NROT),F2INT(6,NROT)
COMMON/SPIN/NC
IF(P.LT.0) RETURN
IF(NC.EQ.1) THEN
BEFF=B(NN,I)*(1.+B(NN,I)/(P*ABS(YE)))
ELSE
BEFF=B(NN,I)*(1.-B(NN,I)/(P*ABS(YE)))
ENDIF
FP=BEFF*R*(R+1)-DE*R**2*(R+1)**2
RETURN
END
REAL FUNCTION FFP(R,NN,IP,P,YY,DEP)
PARAMETER(NROT=125)
COMMON/FACT/F(3,30,30),Y(9,30,2),G(9,30),
1 B(9,30),DG(9,30)
COMMON/F /TR(6,30,30),P1(6,NROT),P2(6,NROT),
1 P1INT(6,NROT),F2INT(6,NROT)
COMMON/SPIN/NC
IF(R.LT.0) RETURN
IF(NC.EQ.1) THEN
BEFF=B(NN-1,IP)*(1.+B(NN-1,IP)/(P*AES(YY)))
ELSE
BEFF=B(NN-1,IP)*(1.-B(NN-1,IP)/(P*AES(YY)))
ENDIF
FPF=BEFF*R*(R+1)-DE*R**2*(R+1)**2
C IF(N.EQ.2) THEN
C WRITE(6,*) 'N,NN,I,B(NN,I),B(NN-1,IP),F,PF'
C WRITE(6,*) N,NN,I,B(NN,I),B(NN-1,IP),R,PF
C ENDF
RETURN
END
REAL FUNCTION XI(N,NN,I,IP,SJ,FR,R,EXPV,YY)
COMMON/FACT/F(3,30,30),Y(9,30,2),G(9,30),
1 B(9,30),DG(9,30)
COMMON/TEMP/TV,TR
COMMON/PERT/IFFERT,TRP,IFPUB,VAR,VAR1,VAR2
DATA P,DE /1,1.2E-6/
IF(R.GE.0) THEN
XI=B(NN,I)/TR*SJ*FR**3*F(N,I,IP)*
1 EXP(-B(NN,I)*R*(R+1)/TR)*EXPV
ELSE
XI=0
ENDIF
C DUE TO PERHAPS A SLOWLY RELAXING NASCENT DIST. OR PERHAPS
C DUE TO CURVE CROSSLINGS(?) AT R VALUES GREATER THAN APPROXIMATELY
C 50 (SEE JEFFERIES) IN V' = C,1 WE SEE ADDITIONAL PCFULATIONS
C IN THE HIGHER ROTATIONAL LEVELS. THIS EFFECT IS APPROXIMATED BY:
IF(IFFERT.EQ.1) THEN
IF(I.LE.2.AND.R.GE.VAR1) THEN
XI=XI+VAR*E(NN,I)/TRP*SJ*FR**3*F(N,I,IP)*
1 EXP(-B(NN,I)*(R-VAR2)*(R-VAR2+1)/TRP)*EXPV
ENDIF
ENDIF
C IF(N.EQ.2) THEN
C WRITE(6,*) 'N,NN,I,B(NN,I),SJ,FR,F(N,I,IP),EXPV,R'

```

```

C      WRITE(6,*) N,NN,I,B(NN,I),SJ,FR,F(N,I,IP),EXPV,R
C      ENDIF
C      RETURN
C      END

C
C      SUBROUTINE AINT(SJ,P,R,Z,Y,RE,PE,ZE,YE)
C THIS SUBROUTINE CALCULATES THE ROTATIONAL LINE STRENGTHS FOR
C DOUBLET TRANSITIONS.
C DEFINITION OF SYMBOLS IN AINT SUBROUTINE:
C INPUT CONSTANTS (LCWER STATE IS A SINGLE LETTER: EXCITED STAT
C HAS AN ADDED E):
C   R,RE - ROTATIONAL QUANTUM NUMBER, J (POSITIVE HALF INTEGER).
C           SELECTION RULE:  $DJ=0,1,-1$ 
C   P,PE - ANGULAR MOMENTUM OF ELECTRONIC STATE, LAMDA (POSITIVE
C           INTEGER OR ZERO). SELECTION RULE:  $DLAMDA=C,1,-1$ 
C   Z,ZE - TOTAL ANGULAR MOMENTUM OF THE ELECTRONS, CMEGA
C           (HALF INTEGER = LAMDA + CR - .5)
C   Y,YE - DIMENSIONLESS SPIN ORBIT COUPLING CONSTANT, LAMDA.
C           PURE CASE A, LAMDA=10000. PURE CASE B, LAMDA<E-5.
C OUTPUT:
C   SJ - ROTATIONAL LINE STRENGTH FACTOR
C
C      SJ=0.0
C      SL=P-PE
C      IF (ABS(SL)-1.01) 1,1,35
1     SR=R-RE
C      IF (ABS(SR)-1.01) 2,2,35
2     IF (ABS(Y)-9999.0) 5,5,3
3     IF (ABS(YE)-9999.0) 13,13,4
4     IF (ABS(Z-ZE)-.01) 13,13,35
5     IF (ABS(Y)-.00002) 6,6,13
6     IF (ABS(YE)-.00002) 7,7,13
7     IF (ABS(R-Z)-.01) 10,10,8
8     IF (ABS(RE-ZE)-.01) 10,10,9
9     IF (ABS(SR-SL+Z-ZE)-1.01) 10,10,35
10    IF (P-.01) 11,11,13
11    IF (PE-.01) 12,12,13
12    IF (ABS(SR+Z-ZE)-.01) 35,35,13
13    IF (R-Z+.01) 35,14,14
14    IF (RE-ZE+.01) 35,15,15
15    AJ=RE+1.0
C      S=P-.5
C      SE=PE-.5
16    IF (ABS(SL)-.01) 23,17,17
17    IF (ABS(SR)-.01) 18,21,21
18    Q=.5*SQRT((AJ+SL*SE)*(RE-SL*SE)
1     *(RE+AJ)/(RE*AJ))
C      GO TO 27
19    Q=.5*SQRT((AJ+1.+SL*SE)*(AJ+SL*SE)/AJ)
C      GO TO 27
20    Q=SE*SQRT((AJ+RE)/(RE*AJ))
C      GO TO 27
21    IF (SR) 22,19,19
22    Q=.5*SQRT((RE-SL*S)*(AJ-SL*S)/RE)
C      GO TO 27
23    IF (ABS(SR)-.01) 20,24,24
24    IF (SR) 26,26,25
25    Q=SQRT((AJ*AJ-SE*SE)/AJ)
C      GO TO 27
26    Q=SQRT((RE*RE-S*S)/RE)

```

```

27  SI=1.0
    SK=1.0
    SIE=1.C
    SKE=1.C
    IF(ABS(Z-S)-.01)30,30,28
28  SI=-1.C
    IF(Z-S+.01)29,29,30
29  SK=-1.C
30  IF(ABS(ZE-SE)-.C1)33,33,31
31  SIE=-1.C
    IF(ZE-SE+.C1)32,32,33
32  SKE=-1.C
33  S=S+1
    SE=SE+1
    SJ=SJ+T(SI,SK,P,R,Y)*Q*T(SIE,SKE,PE,RE,YE)
    IF(S-P-1.49)16,34,34
34  SJ=SJ*SJ
35  RETURN
    END
    REAL FUNCTION T(SI,SK,P,R,Y)
    IF(P-.C1)6,6,1
1   IF(R+.49-P)9,9,2
2   AJ=2.*R+1.
    IF(ABS(Y)-.C00C2)8,8,3
3   SL=Y/AES(Y)
    IF(ABS(Y)-9999.C)4,4,7
4   GA=Y*P*P/AJ-R-.5
    GB=.5*SQRT(AJ**2+Y*(Y-4.)*F*P)
5   BK=1./SQRT(2.*GE*AJ)
    T=BK*(SQRT((GB-SI*GA)*(R+.5-SL*P)))+SI
1  *SQRT((GB+SI*GA)*(R+.5+SL*P)))*SK
    GO TO 10
6   T=SI/SQRT(2.0)*SK
    GO TO 10
7   GA=SL*P*P/AJ
    GB=.5*P
    GO TO 5
8   T=SI*SK*SQRT((R+.5-SI*P)/AJ)
    GO TO 10
9   T=.5*SK*(1.+SI)
10  RETURN
    END
    SUBROUTINE LORNTZN(N,I,IP)
    PARAMETER(NROT=125)
    COMMON/FACT/F(3,30,30),Y(9,30,2),G(9,30),
1  9(9,30),DG(9,30)
    COMMON/P /TR6(6,30,30),P1(6,NROT),P2(6,NROT),
1  P1INT(6,NROT),P2INT(6,NROT)
    COMMON/G /Q1(6,NROT),Q2(6,NROT),
1  Q1INT(6,NROT),Q2INT(6,NROT)
    COMMON/R /R1(6,NROT),R2(6,NROT),R1INT(6,NROT),
1  R2INT(6,NROT),FINT(6,1C00C),FIN(1CCCC),FINX(1CCCC)
    COMMON/TEMP/TV,TR
    COMMON/INPUT/NTITLE,IFDIS,IERANCH,WPIN,WMAX,RRES,
1  XTV,XTR,IFDNE,IFDEF,IPIN,IMAX,IENVH,ENVH1,V,
2  XP,TK,GAMPA2
    COMMON/INDEX/NF,NF1,NF2,NT,ND,ND1
    COMMON/PEAK/XPEAK(6,30,30),YPEAK(6,30,30),FCH(1C00C)
    CHARACTER*4C NTITLE

```

```

C      NORMALIZED LORENTZIAN--SLIGHT REDISTRIBUTION OF
C      INTENSITIES
C
C      GAMMA2=3.16E13*3.16E13
      IDIF=IPAX-IMIN
      IXN=3
      WIL=1.E8/TRW(N,I,IF)
      IF(WIL.LT.4*MIN+ENVH) THEN
      IL=INT((WIL+.1*FRES)/RRES)-IMIN+1
      IU=IL+IENVH
      XN=WIL
      ELSE
      IL=INT((WIL+.1*FRES)/RRES)-IMIN-IENVH+1
      IU=IL+2*IENVH
      XN=WIL-IENVH*RRES
      ENDIF
      WRITE (3,*) 'IL=',IL,'IU=',IU
      FMAX=C
      FMAX1=C
      FMAXCLD=0
      FMP=C
      RR=0.
      DO 110 I1=IL,IU
      IF(I1.LT.1.CR.I1.GT.IDIF)GO TO 110
      RR=RR+RRES
      XI1=XN+RR
C      XI1I=3.E18/XI1
      SUM=C
      IF(N.EG.1) THEN
      DO 120 J=1,NRCT
      DENOM=(XI1-1.E8/F1(N,J))*+2+GAMMA2
      SC=GAMMA2/DENOM
      SUP=SUM+SC*P1INT(N,J)
120    CONTINUE
      DO 130 J=1,NROT
      DENOM=(XI1-1.E8/R1(N,J))*+2+GAMMA2
      SC=GAMMA2/DENOM
      SUP=SUM+SC*R1INT(N,J)
130    CONTINUE
      DO 140 J=1,NRCT
      DENOM=(XI1-1.E8/Q1(N,J))*+2+GAMMA2
      SC=GAMMA2/DENOM
      SUP=SUM+SC*Q1INT(N,J)
140    CONTINUE
      ELSE
      DO 150 J=1,NRCT
      DENOM=(XI1-1.E8/P2(N,J))*+2+GAMMA2
      SC=GAMMA2/DENOM
      SUP=SUM+SC*P2INT(N,J)
150    CONTINUE
      DO 160 J=1,NRCT
      DENOM=(XI1-1.E8/R2(N,J))*+2+GAMMA2
      SC=GAMMA2/DENOM
      SUP=SUM+SC*R2INT(N,J)
160    CONTINUE
      DO 170 J=1,NRCT
      DENOM=(XI1-1.E8/G2(N,J))*+2+GAMMA2
      SC=GAMMA2/DENOM
      SUP=SUM+SC*G2INT(N,J)
170    CONTINUE

```

```

ENDIF
FIN(I1)=FIN(I1)+SUM
FCH(I1)=SUM
C   WRITE(6,*) 'DEN=',DENCM,SC,GAMMA2,Q2INT(N,J),SUM
C   FIND THE MAX Y POSITION OF "CLOSE" PEAKS
FMAX=MAX(FIN(I1),FMAX)
FMAX1=MAX(FCH(I1),FMAX1)
IF(FMAX.GT.FMAXOLD.AND.(FMAX1/FMAX).GT..2) THEN
FMAXOLD=FMAX
YPEAK(N,I,IP)=MAX(YPEAK(N,I,IP),FMAX)
ENDIF
110 CONTINUE
C
C   END OF INTEGRATION
C
C
C   FIND THE PEAK OF EACH SPECTRUM LINE
C
FMAX=0
FMAX1=0
FMAXOLD=0
RR=0.
IL=INT((WIL+.1*FRES)/RRES)-IMIN-IXN+1
IU=IL+2*IXN
XN=WIL-IXN*RRES
DO 5 I1=IL,IU
IF(I1.LT.1.OR.I1.GT.IDIF)GO TO 5
RR=RR+RRES
XI1=XN+RR
FMAX=MAX(FIN(I1),FMAX)
FMAX1=MAX(FCH(I1),FMAX1)
IF(FMAX.GT.FMAXOLD.AND.(FMAX1/FMAX).GT..2) THEN
XPEAK(N,I,IP)=XI1
YPEAK(N,I,IP)=MAX(YPEAK(N,I,IP),FMAX)
FMAXOLD=FMAX
ENDIF
5 CONTINUE
RETURN
END
SUBROUTINE GAUSSN(N,I,IP)
PARAMETER(NROT=125)
COMMON/FACT/F(3,30,30),Y(9,30,2),G(9,30),
1 B(9,30),DG(9,30)
COMMON/P /TRW(6,30,30),P1(6,NROT),P2(6,NROT),
1 P1INT(6,NROT),P2INT(6,NROT)
COMMON/G /Q1(6,NROT),G2(6,NROT),
1 Q1INT(6,NROT),G2INT(6,NROT)
COMMON/R /R1(6,NROT),R2(6,NROT),R1INT(6,NROT),
1 R2INT(6,NROT),FINT(6,1000),FIN(1000),FINX(1000)
COMMON/TEMP/TV,TR
COMMON/INPUT/NTITLE,IFDIS,IBRANCH,IPIN,IMAX,RRES,
1 XTV,XTR,IFDONE,IFDEF,IPIN,IMAX,IENVH,ENVH1,V,
2 XP,TK,GAMMA2
COMMON/INDEX/NF,NF1,NF2,NT,ND,ND1
COMMON/PEAK/XPEAK(6,30,30),YPEAK(6,30,30),FCH(1000)
CHARACTER*4C NTITLE
C
C   NORMALIZED GAUSSIAN
C
RETURN

```

```

END
SUBROUTINE OUTPLT
PARAMETER(NROT=125)
COMMON/FACT/F(3,30,30),Y(9,30,2),G(9,30),
1 B(9,30),DG(9,30)
COMMON/P /TRW(6,30,30),P1(6,NROT),P2(6,NROT),
1 P1INT(6,NROT),P2INT(6,NROT)
COMMON/G /Q1(6,NROT),Q2(6,NROT),
1 Q1INT(6,NROT),Q2INT(6,NROT)
COMMON/R /R1(6,NROT),R2(6,NROT),R1INT(6,NROT),
1 R2INT(6,NROT),FIN(6,1000),FIA(1000),FIAX(1000)
COMMON/TEMP/TV,TR
COMMON/INPLT/NTITLE,IFDIS,IERANCH,WMIN,WMAX,RRES,
1 XTV,XTR,IFDNE,IFDEF,IPIN,IMAX,IENVH,ENVH1,V,
2 XP,TK,GAMMA2
COMMON/INDEX/NF,NF1,NF2,NT,ND,ND1
COMMON/PEAK/XPEAK(6,30,30),YPEAK(6,30,30),FCH(1000)
COMMON/WGHT/WGHT(30,30),NVIS,IFEXCIT
COMMON/CNTR/CNTR(3,30,30),IFCENTR
COMMON/EXPDAT/IFDATA,WAVE(20,1030),SPEC(20,1030),WAV(2000),
1 SF(2000),WW(2000),SPW(2000),WDAT(20),SEN(20),ICCNT,IIMAX,
2 INMAX,EKGRND,SLOPE
COMMON/FERT/IFFERT,TRP,IFPLE,VAR,VAR1,VAR2
DIMENSION FINY(1000),YMAXX(30,30)
CHARACTER*4C NTITLE

```

C
C

```
CALL ASSIGN(7,'OUTPUT.SPEC')
```

C
C
C

```
WRITE INPUT FILE FOR CONTINUATION RUNS
```

```

CALL ASSIGN(2,'INPUT.DAT')
WRITE(2,*) WMIN,WMAX,RRES,XTV,XTR
WRITE(2,35) NTITLE
35  FORMAT(A30)
WRITE(2,*) IFDIS,IERANCH,ENVH1,TK,XP,GAMMA2
WRITE(2,*) IFEXCIT,IFCENTR
CALL CLOSE(2)

```

C
C
C

```
NORMALIZE INTENSITY
```

```

YMAX=0.
YMIN=1.E20
LMN=IMAX-IPIN
LMNN=LMN-2*IENVH
C  DO 10 I=1,LMNN
DO 10 I=IENVH,LMN-IENVH
YMAX=MAX(FIN(I),YMAX)
YMIN=MIN(FIN(I),YMIN)
10  CONTINUE
YM=YMAX
II=0
WMEN=WMIN-ENVH1
C  DO 20 I=1,LMNN
DO 20 I=IENVH,LMN-IENVH
II=II+1
FINX(II)=WMEN+FLOAT(I-1)*RRES
FINY(II)=FIN(I)/YMAX
WRITE(7,*) FINX(II),FINY(II)

```

```

20    CONTINUE
C
C    NORMALIZE PEAK INTENSITIES
C
      DO 25 N=1,NT
      DO 24 I=1,NF1
      DO 23 IP=1,NF2
      YPEAK(N,I,IP)=YFEAK(N,I,IP)/YMAX
23    CONTINUE
24    CONTINUE
25    CONTINUE
      YMIN=YMIN/YMAX
      YMAX=1.

C
C    PLOT THE INTENSITY SPECTRUM AS A FUNCTION OF WAVELENGTH IN
C    ANGSTROMS USING DISPLA.
C
      TTV=TV/.695
      TTR=TR/.695
C
      XLWAV=WMIN-ENVH1
C
      XLWAV1=WMAX+ENVH1
      XLWAV=WMIN
      XLWAV1=WMAX
      CALL PAGE(11,8.5)
      CALL AREA2D(10,6.5)
      NCHAR=INDEX(NTITLE,' ')
      CALL HEADIN(XREF(NTITLE),NCHAR,2.,1)
      CALL XNAME('WAVELENGTH (ANGSTROMS)',100)
      CALL YNAME('NORMALIZED INTENSITY',100)
      CALL GRAF(XLWAV,'SCALE',XLWAV1,YMIN,'SCALE',YMAX)
      CALL MESSAG('RCT TEMP=',100,7.35,6.25)
      CALL REALNC(TTR,-4,'ABUT','ABUT')
      CALL DASH
      CALL CURVE(FINX,FINY,LMNN,C)
      CALL RESET('DASH')
      WRITE(3,*)'IFDATA,IFEXCIT=',IFDATA,IFEXCIT
      IF(IFEXCIT.EQ.C)THEN
        NVIB=12
        CALL MESSAG('VIB TEMP=',100,7.35,6.0)
        CALL REALNC(TTV,-4,'ABUT','ABUT')
        IF(IFDATA.EQ.C) THEN
          CALL MESSAG('V 1/2-1/2PCF 3/2-3/2POP',100,7.35,5.75)
          YPOS=5.5
          DO 200 JJ=1,NVIB
          XPOS=7.35
          CALL INTNC(JJ-1,XPCS,YPOS)
          XPOS=XPCS+.3125
          CALL REALNC(WGHT(1,JJ),-2,XPCS,YPCS)
          XPOS=XPOS+1.3
          CALL REALNC(WGHT(2,JJ),-2,XPCS,YPCS)
          YPOS=YPOS-.2
200    CONTINUE
          ELSE
          CALL MESSAG('-- SYNTHETIC SPECTRUM',100,7.35,5.75)
          CALL MESSAG('V 1/2-1/2PCF 3/2-3/2POP',100,7.35,5.25)
          YPCS=5.0
          DO 210 JJ=1,NVIB
          XPCS=7.35
          CALL INTNC(JJ-1,XPOS,YPOS)
          XPOS=XPOS+.3125

```

```

CALL REALNO(WGHT(1,JJ),-2,XPCS,YPCS)
XPOS=XPOS+1.3
CALL REALNO(WGHT(2,JJ),-2,XPCS,YPOS)
YPOS=YPOS-.2
210 CONTINUE
IF(IFPUB.EQ.C) THEN
CALL SETCLR('RED')
ENDIF
CALL MESSAGE(' - EXPER. SPECTRUMS',100,7.35,5.5)
C CALL MARKER(15)
C CALL SCLPIC(.7)
C CALL CURVE(WW,SPW,INMAX,INMAX/100)
CALL CURVE(WW,SPW,INMAX,C)
WRITE(7,*) 'EXP WAVELENGTH , EXP PHOTON COUNTS'
DO 27 II=1,INMAX
WRITE(7,*) WW(II),SPW(II)
27 CONTINUE
ENDIF
ENDIF
IF(IFEXCIT.EQ.1) THEN
IF(IFDATA.EQ.C) THEN
CALL MESSAGE('V 1/2-1/2PCP 3/2-3/2PCP1',100,7.35,6.0)
YPOS=5.75
DO 300 JJ=1,NVIB
XPOS=7.35
CALL INTAC(JJ-1,XPOS,YPOS)
XPOS=XPOS+.3125
CALL REALNO(WGHT(1,JJ),-2,XPCS,YPCS)
XPOS=XPOS+1.3
CALL REALNO(WGHT(2,JJ),-2,XPCS,YPOS)
YPOS=YPOS-.2
300 CONTINUE
ELSE
CALL MESSAGE('-- SYNTHETIC SPECTRUMS',100,7.35,6.0)
CALL MESSAGE('V 1/2-1/2PCP 3/2-3/2PCP1',100,7.35,5.5)
YPOS=5.25
DO 310 JJ=1,NVIB
XPCS=7.35
CALL INTAC(JJ-1,XPOS,YPOS)
XPOS=XPOS+.3125
CALL REALNO(WGHT(1,JJ),-2,XPCS,YPCS)
XPOS=XPOS+1.3
CALL REALNO(WGHT(2,JJ),-2,XPCS,YPCS)
YPOS=YPOS-.2
310 CONTINUE
IF(IFPUB.EQ.C) THEN
CALL SETCLR('RED')
ENDIF
CALL MESSAGE(' - EXPER. SPECTRUMS',100,7.35,5.75)
C CALL MARKER(15)
C CALL SCLPIC(.7)
CALL CURVE(WW,SPW,INMAX,C)
WRITE(7,*) 'EXP WAVELENGTH , EXP PHOTON COUNTS'
DO 127 II=1,INMAX
WRITE(7,*) WW(II),SPW(II)
127 CONTINUE
ENDIF
ENDIF
CALL HEIGHT(.02)
CALL ANGLE(90.)

```

```

      XN=1.7*.007353*(WMAX-WMIN)
      YN=.025
      CALL SETCLR('BLLE')
C     FIND WHERE LINE TRANSITION NUMBERS WILL OVERLAP AND ELLIMNATE THE
C     OVERLAPPING NUMBERS
      N=1
      NN=2
      DO 40 I=1,NF1
      DO 50 IP=1,NF2
        IF(AES(XPEAK(N,I,IP)-XPEAK(NN,I,IP)).LT.XN)THEN
          WRITE(3,*) 'ABS(XP1/2-XF3/2),XN,I,IF=',ABS(XPEAK(N,I,IP)-
1          XPEAK(NN,I,IP)),XN,I,IP
          YPEAK(NN,I,IF)=YPEAK(NN,I,IF)+1C
          WRITE(3,*) 'YPEAK(2,I,IF)=',YPEAK(NN,I,IP)
          ENDIF
50      CONTINUE
40      CONTINUE
C     WRITE THE NON-OVERLAPPING NUMBERS ON THE PLCT
      N=1
      DO 60 I=1,NF1
      DO 70 IP=1,NF2
        IF(XLWAV.GT.XPEAK(N,I,IP).CR.XLWAV1.LT.XPEAK(N,I,IP))
1      GO TC 70
        IF(YPEAK(N,I,IP).LT..001) GO TC 7C
        IC=I-1
        IPO=IP-1
        XMESS=XPEAK(N,I,IF)
        YMESS=1.+YN
        CALL RLMESS('(',1,XMESS,YMESS)
        CALL RLINT(10,'ABLT','ABUT')
        CALL RLMESS(')',1,'ABUT','ABUT')
        CALL RLINT(IPC,'AEUT','ABUT')
        CALL RLMESS(')1/23',10C,'AEUT','ABUT')
70      CONTINUE
60      CONTINUE
      N=2
      DO 80 I=1,NF1
      DO 90 IP=1,NF2
        IF(XLWAV.GT.XPEAK(N,I,IP).CR.XLWAV1.LT.XPEAK(N,I,IP))
1      GO TC 90
        IF(YPEAK(N,I,IP).LT..001) GO TC 9C
        IF(YPEAK(N,I,IP).LT.8) THEN
          IC=I-1
          IPO=IP-1
          XMESS=XPEAK(N,I,IF)
          YMESS=1.+YN
          CALL RLMESS('(',1,XMESS,YMESS)
          CALL RLINT(IC,'ABLT','ABUT')
          CALL RLMESS(')',1,'ABUT','ABUT')
          CALL RLINT(IPC,'AEUT','ABLT')
          CALL RLMESS(')1/23',10C,'AEUT','ABUT')
        ENDIF
90      CONTINUE
80      CONTINUE
      CALL RESET('HEIGHT')
      CALL RESET('ANGLE')
      CALL ENDPL(-1)
C
      RETURN
      END

```

```

SUBROUTINE PLTDEV (NAMDEV)
*****
*
*               (DEFINE   SUBROUTINE   HERE   !!!)
*
*****
*
*   WRITTEN BY:
*
*
*               FRANK J. SEILER RESEARCH LABCRATCRY
*               UNITED STATES AIR FORCE ACADEMY
*               COLORADO SPRINGS, COLORADO 80840
*
*****
*   INPUT PARAMETERS:
*   NAMDEV - OUTPUT DEVICE CHOSEN BY USER
*-----
*   CHARACTER*45 NAMDEV
*****
*   LOCAL VARIABLES:
*   IBUF -
*   IERR - ERROR NUMBER
*-----
*   INTEGER IBUF,I,II,IERR
*   DIMENSION IBUF(16)
*****
*   CHARACTER BELL
*   BELL = CHAR(7)
*   TERMINAL DEVICES
*   IF (NAMDEV .EQ. 'VT 240') GOTO 2100
*   IF (NAMDEV .EQ. 'TEKTRONIX 4107') GOTO 2200
*   IF (NAMDEV .EQ. 'TEKTRONIX 4010') GOTO 2300
*   IF (NAMDEV .EQ. 'VT 100 RETRC') GOTO 2400
*   HARDCOPY DEVICES
*   IF (NAMDEV .EQ. 'PRINTRONICS') GOTO 3100
*   IF (NAMDEV .EQ. 'HP 7550') GOTO 3200
*   IF (NAMDEV .EQ. 'HP 7475') GOTO 3300
*   IF (NAMDEV .EQ. 'ANY ASCII PRINTER') GOTO 3400
*   IF (NAMDEV .EQ. 'POST PROCESSOR') GOTO 4100
*   ERROR, QUIT
*   GOTO 9100
*-----
*   TERMINAL DEVICES
*-----
*   VT 240

2100 CONTINUE

*   SET CONFIGURATION TO STANDARD I/O
*   IBUF(1)=C
*   CALL IOMGR(IBUF,-102)

*   CALL VT240

*   GOTO 99000
*-----
*   TEKTRONIX 4107

2200 CONTINUE

```

```

*   SET CONFIGURATION TO STANDARD I/O
    IBUF(1)=C
    CALL IOMGR(1BLF,-102)

    CALL TK41 (41C7)

*   PLOT ORIENTATION -      AUTO : AUTO ACCORDING TO PLT SIZE
*                           CCMIC: X AXIS HORIZONTAL
*                           PCVIE: Y AXIS HORIZONTAL
C   CALL HWROT('CCMIC')

    GOTO 99000
-----
*   TEKTRONIX 401C

2300   CONTINUE

    CALL P401C

    GOTO 99000
-----
*   VT 102 WITH GRAPHICS RETRCFIT

2400   CONTINUE
*   SET CONFIGURATION TO STANDARD I/O
*   IBUF(1)=C
    CALL IOMGR(1ELF,-102)

    CALL PDEV1

    GOTO 99000
-----
*
2500   CONTINUE

    GOTO 99000
-----
*
2600   CONTINUE

    GOTO 99000
-----
*
2700   CONTINUE

    GOTO 99000
-----
*   HARDCCPY DEVICES
*   PRINTRCNICS

3100   CONTINUE

    CALL PPNTNX

    GOTO 99000
-----

```

* HP 7550

3200 CONTINUE

* SET CONFIGURATION TO SPOOL
IBUF(1)=5
CALL IOMGR(IELF,-102)

* SET FILE OPEN MODE
* 3 - NO CVERWRITE, CREATES NEW VERSION NUMBER
* 0 - APPEND TO FILE
IBUF(1)=3
CALL IOMGR(IELF,-104)

* SET PLOT FILE NAME
DO 3220 II=1,16
IBUF(II)=C

3220 CONTINUE

PRINT '(/////)'

3240 CONTINUE

PRINT '(\$\$S\$',

+ ' ENTER PLOT FILE NAME OR Q TO QUIT: ',A)', BELL

READ(5, '(14A4)', ERR=93CC) (IBUF(II), II=1, 14)

C IF (IBUF(1) .EQ.)

CALL IOMGR(IELF,-103)

CALL HP7550 (1)

* PLOT ORIENTATION - AUTO : AUTO ACCORDING TO PLT SIZE
* CCMIC: X AXIS HORIZONTAL
* MOVIE: Y AXIS HORIZONTAL
C CALL HWRCT('MOVIE')

GOTO 99CCC

* HP 7475

3300 CONTINUE

* SET CONFIGURATION TO SPOOL
IBUF(1)=5
CALL IOMGR(IELF,-102)

* SET FILE OPEN MODE
* 3 - NO CVERWRITE, CREATES NEW VERSION NUMBER
* 0 - APPEND TO FILE
IBUF(1)=3
CALL IOMGR(IELF,-104)

* SET PLOT FILE NAME
DO 3320 II=1,16
IBUF(II)=C

3320 CONTINUE

PRINT '(/////)'

3340 CONTINUE

PRINT '(\$\$S\$',

+ ' ENTER PLOT FILE NAME: ',A)', BELL

```

      READ(S, '(14A4)', ERR=94CC) (I9UF(II), II=1, 14)
      CALL ICMGR(IEBF,-103)

      CALL HP7475 (1)

*      PLOT ORIENTATION -      AUTO :  AUTO ACCORDING TO PLT SIZE
*                                  COMIC:  X AXIS HORIZONTAL
*                                  MOVIE:  Y AXIS HORIZONTAL
C      CALL HWRCT('MOVIE')

      GOTO 990CC
*-----
*      ANY ASCII PRINTER

3400      CONTINUE

      CALL FPRTPL

      GOTO 990CC
*-----
*      POST PROCESSOR
*-----
4100      CONTINUE

      CALL COMPRS

      GOTO 990CC
*-----

*      ERROR HANDLING  *****

*      DEVICE SELECTION ERROR  -----
9100      PRINT '(*O*',
+          21X, '  *** ERROR IN PLOT DEVICE SELECTION ***',
+          A, A, A)', BELL, BELL, BELL
      STOP

*      HP 7550 FILE NAME ERROR  -----
9300      PRINT '(*O*',
+          21X, '  *** ERROR IN FILE NAME ***', A, /,
+          21X, '  PRESS RETURN', A, A)', BELL, BELL, BELL
      READ(S, '(I1)', IOSTAT=IERR) I
      GOTO 324C

*      HP 7475 FILE NAME ERROR  -----
9400      PRINT '(*O*',
+          21X, '  *** ERROR IN FILE NAME ***', A, /,
+          21X, '  PRESS RETURN', A, A)', BELL, BELL, BELL
      READ(S, '(I1)', IOSTAT=IERR) I
      GOTO 334C

9900C      CONTINUE
      RETURN
      END

C
C*****
C      SUBROUTINE LCADFIL

C
C      THIS LOADS THE OPA FILES THAT INCLUDE WAVELENGTH INFORMATION

```

C IT ALSO PLACES THE WAVELENGTH AND CORRESPONDING INTENSITY DATA
 C IN FILES TO BE MANIPULATED IN SUBROUTINE SPLICE. IT IS ASSUMED
 C THAT THE CMA FILES TO BE PLOTTED ARE PRESENT IN THE LOCAL FILE
 C SPACE AND LISTED IN FILE FILE.CMA.

C
 COMMON/EXPCAT/IFDATA,WAVE(20,1030),SPEC(20,1030),WAV(20000),
 1 SP(20000),WW(20000),SPW(20000),WDAT(20),SEN(20),ICOUNT,IIMAX,
 2 INMAX,BKGRND,SLOPE
 COMMON/COF/ACOF(20,50)
 CHARACTER*6 SHOTNO, SPC
 CHARACTER*4 END
 CHARACTER*10 SNODAT,FILES
 CHARACTER*20 CDUMMY1,CDUMMY1

C
 C
 DUMMY=0
 ICOUNT=0
 FILES='FILE.CMA'
 CALL ASSIGN(4,FILES)
 WRITE(6,*) 'LOADING FILES (NAMED IN FILE.CMA):'
 DO 100 I=1,20
 READ(4,101,END=9) SHCTNO
 ICOUNT=ICOUNT+1
 WRITE(6,*) I, ' FILE= ',SHCTNO
 INUM=I
 101 FORMAT (A6)
 END='.CMA'
 SNODAT=SHOTNO//END
 CALL ASSIGN(2,SNODAT)
 READ(2,102) CDUMMY1
 102 FORMAT(A19)
 DO 10 II=1,3
 READ(2,103) CDUMMY2
 103 FORMAT(A11)
 10 CONTINUE
 DO 200 J=1,1024
 READ(2,*,END=201) SPEC(I,J)
 200 CONTINUE
 201 CONTINUE
 READ(2,102) CDUMMY1
 DO 20 II=1,3
 READ(2,103) CDUMMY2
 20 CONTINUE
 DO 210 J=1,40
 READ(2,*,END=211) ACCF(I,J)
 210 CONTINUE
 211 CONTINUE
 CALL CLOSE(2)
 C WRITE(3,*) 'EXP WAVE LEN , EXP PHOTON COUNT'
 DO 220 J=1,1024
 WAVE(I,J)=ACCF(I,36)+ACOF(I,37)*(FLOAT(J)-1.)
 C WRITE(3,*) WAVE(I,J),SPEC(I,J)
 220 CONTINUE
 100 CONTINUE
 9 CONTINUE
 CALL CLOSE(4)
 RETURN
 END

C
 SUBROUTINE SPLICE

C THIS SUBROUTINE SPLICES TOGETHER CMA FILES. IT IS ASSUMED
C THAT THE DATA FILES OVERLAP EACH OTHER AND THAT THEY ARE
C NAMED IN FILE FILE.CMA. IT IS ALSO ASSUMED THAT THE FIRST FILE
C NAMED CORRESPONDS TO THE SHORTEST WAVELENGTH AND SC ON.

```

C      COMMON/EXPCAT/IFDATA,WAVE(20,1030),SPEC(20,1030),WAV(20000),
1      SP(20000),WW(20000),SPW(20000),WDAT(20),SEN(20),ICOUNT,IIMAX,
2      INMAX,BKGRND,SLOPE
      COMMON/COF/ACCF(20,50)
      DC 20 I=1,ICOUNT
        IF(I.EQ.1) THEN
          IC=1
          X=ACCF(I,36)
        ELSE
          IC=ICOLD-INT((WMAXOLD-ACCF(I,36))/DXCLD)
          X=X-(WMAXOLD-ACCF(I,36))
        ENDIF
        WRITE(3,*) 'ACCF(I,36)=',ACCF(I,36),'ACCF(I,37)=',ACCF(I,37)
        WRITE(3,*) 'IC,X,WMAXOLD,ICOLD,DXCLD=',IC,X,WMAXOLD,ICOLD,
1          DXCLD
      DC 30 II=1,1024
        WAV(IC)=X
        SP(IC)=MAX(SP(IC),SPEC(I,II))
        X=X+ACCF(I,37)
        IC=IC+1
30      CONTINUE
        WMAXOLD=X-ACCF(I,37)
        ICOLD=IC-1
        DXCLD=ACCF(I,37)
20      CONTINUE
        IIMAX=ICOLD
      END
      SUBROUTINE WEIGHT(WMIN,WMAX)

```

C THIS ROUTINE WEIGHTS THE SPECTRAL COUNTS WITH THE INVERSE OF
C THE CMA SENSITIVITY. IT ALSO NORMALIZES THE EXPERIMENTAL SPECTRA
C AND LOADS THE FINAL PLOTTING ARRAYS.

```

C      COMMON/EXPCAT/IFDATA,WAVE(20,1030),SPEC(20,1030),WAV(20000),
1      SP(20000),WW(20000),SPW(20000),WDAT(20),SEN(20),ICOUNT,IIMAX,
2      INMAX,BKGRND,SLOPE
      DATA WDAT / 250.,260.,270.,280.,290.,300.,320.,350.,370.,400.,
1      450.,500.,550.,600.,650.,700.,750.,800.,900.,1000/
C      DATA SEN / 2.89,3.16,3.32,4.26,5.22,4.2,5.53,5.55,5.04,6.1,
C      1      8.24,11.73,17.81,29.7,49.7,57.03,117.,237.,513.7,
C      1      787.97/
      DATA SEN / .529,.576,.6,.634,.672,.755,.956,1.06,.972,1.00,
1      1.35,1.94,2.99,4.93,8.0,9.5,19.34,37.93,1038,1669/
C
      WWPIN=WMIN/10.
      WWMAX=WMAX/10.
      II=0
      SPWMAX=1E-20
      WRITE(3,*) 'IIMAX=',IIMAX
      DO 100 I=1,IIMAX
C      WRITE(3,*) 'WWPIN,WWMAX,WAV=',WWPIN,WWMAX,WAV(I)
        IF(WAV(I).LT.WWPIN.OR.WAV(I).GT.WWMAX) GO TO 110
        J=C
        II=II+1
        IF(WAV(I).LT.WDAT(1)) THEN

```

```

      WT=SEN(1)
    ELSE IF(WAV(I).LT.WDAT(2)) THEN
      J=2
      WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
1      (WDAT(J)-WDAT(J-1))
    ELSE IF(WAV(I).LT.WDAT(3)) THEN
      J=3
      WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
1      (WDAT(J)-WDAT(J-1))
    ELSE IF(WAV(I).LT.WDAT(4)) THEN
      J=4
      WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
1      (WDAT(J)-WDAT(J-1))
    ELSE IF(WAV(I).LT.WDAT(5)) THEN
      J=5
      WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
1      (WDAT(J)-WDAT(J-1))
    ELSE IF(WAV(I).LT.WDAT(6)) THEN
      J=6
      WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
1      (WDAT(J)-WDAT(J-1))
    ELSE IF(WAV(I).LT.WDAT(7)) THEN
      J=7
      WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
1      (WDAT(J)-WDAT(J-1))
    ELSE IF(WAV(I).LT.WDAT(8)) THEN
      J=8
      WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
1      (WDAT(J)-WDAT(J-1))
    ELSE IF(WAV(I).LT.WDAT(9)) THEN
      J=9
      WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
1      (WDAT(J)-WDAT(J-1))
    ELSE IF(WAV(I).LT.WDAT(10)) THEN
      J=10
      WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
1      (WDAT(J)-WDAT(J-1))
    ELSE IF(WAV(I).LT.WDAT(11)) THEN
      J=11
      WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
1      (WDAT(J)-WDAT(J-1))
    ELSE IF(WAV(I).LT.WDAT(12)) THEN
      J=12
      WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
1      (WDAT(J)-WDAT(J-1))
    ELSE IF(WAV(I).LT.WDAT(13)) THEN
      J=13
      WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
1      (WDAT(J)-WDAT(J-1))
    ELSE IF(WAV(I).LT.WDAT(14)) THEN
      J=14
      WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
1      (WDAT(J)-WDAT(J-1))
    ELSE IF(WAV(I).LT.WDAT(15)) THEN
      J=15
      WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
1      (WDAT(J)-WDAT(J-1))
    ELSE IF(WAV(I).LT.WDAT(16)) THEN
      J=16
      WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/

```

```

1      (WDAT(J)-WDAT(J-1))
ELSE IF(WAV(I).LT.WDAT(17)) THEN
  J=17
  WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
1      (WDAT(J)-WDAT(J-1))
ELSE IF(WAV(I).LT.WDAT(18)) THEN
  J=18
  WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
1      (WDAT(J)-WDAT(J-1))
ELSE IF(WAV(I).LT.WDAT(19)) THEN
  J=19
  WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
1      (WDAT(J)-WDAT(J-1))
ELSE IF(WAV(I).LT.WDAT(20)) THEN
  J=20
  WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
1      (WDAT(J)-WDAT(J-1))
ELSE IF(WAV(I).GT.WDAT(20)) THEN
  WT=SEN(20)
ENDIF
C SHIFT EXP. SPECTRA TO LEFT BY 6 ANGSTROMS DUE EXP. CAL. ERROR
WW(II)=WAV(I)*10.-6
SPW(II)=SP(I)*WT-(EKGRND+SLCPE*(WW(II)-WMIN))
C      SPW(II)=SF(I)*WT
C      ELLIMINATE NH PEAK FROM DATA NORMALIZATION--OR OTHER PEAKS IF
C      SC DESIRED.
      IF(3345.LT.WW(II).AND.3375.GT.WW(II)
1      .CR.5250.LT.WW(II).AND.5340.GT.WW(II)) THEN
C      DC NOTHING
      ELSE
        SPWMAX=MAX(SPW(II),SPWMAX)
      ENDIF
110  CONTINUE
100  CONTINUE
      INMAX=II
      WRITE(3,*) 'INMAX=',INMAX
C      NORMALIZE THE EXPERIMENTAL SPECTRA TO THE HIGHEST NON-
C      EXCLUDED PEAK
      DO 200 I=1,INMAX
        SPW(I)=SPW(I)/SPWMAX
C        WRITE(3,*) 'WV,SPW=',WV(I),SPW(I)
200  CONTINUE
C      CHOP OFF UNWANTED LINES EXTENDING OUTSIDE OF THE PLOTTING
C      AREA
      DO 210 I=1,INMAX
        IF(SPW(I).GT.1.(1)SPW(I)=1.
210  CONTINUE
      RETURN
      END

```

2	7	10	2
.C028	.0193	.0637	.1315
.0137	.0658	.1329	.1365
.C357	.1121	.1178	.C3C3
.C656	.1238	.0458	.0C48
.C952	.0951	.0015	.0537
.1164	.0484	.C143	.0695
.1249	.0119	.C496	.0343
.C031	.0211	.C679	.1369
.C153	.0707	.1373	.1342
.C395	.1176	.1151	.0246
.C717	.1253	.C392	.0C84
.1027	.0908	.C002	.C6C5
.1236	.0413	.C208	.0679
.130C	.0C72	.0573	.C270

Franck-Condon Factors (File: FRANK.CON)

1.5951	1.6164	1.6383	1.6607	1.6837	1.7074	1.7320	1.7410	1.741C	1.741C
1.5811	1.6019	1.6230	1.6444	1.6656	1.6716	1.7186	1.7410	1.741C	1.741C
1.5676	1.5877	1.6080	1.6273	1.6588	1.6758	1.6972	1.7169	1.741C	1.741C
1.5544	1.574C	1.5930	1.6229	1.6379	1.6575	1.5644	1.7C78	1.729C	1.741C
1.5417	1.56C6	1.5699	1.6C30	1.6216	1.7599	1.6679	1.6872	1.5298	1.7398
1.5293	1.5472	1.5715	1.5882	1.60C5	1.6318	1.6498	1.7C60	1.6977	1.7164
1.5172	1.5331	1.5567	1.5736	1.5997	1.6155	1.6C72	1.66C1	1.6771	1.7139
1.5886	1.61C2	1.6322	1.6548	1.678C	1.7018	1.7265	1.741C	1.741C	1.741C
1.5744	1.5955	1.6168	1.6384	1.6596	1.646C	1.7126	1.7357	1.741C	1.741C
1.56C6	1.5812	1.6C17	1.6209	1.6513	1.6698	1.6914	1.71C3	1.741C	1.741C
1.5472	1.5672	1.5864	1.6145	1.6316	1.6513	1.7186	1.7C17	1.7231	1.741C
1.5342	1.5536	1.5473	1.5963	1.6151	1.6579	1.6616	1.68C9	1.7485	1.7336
1.5215	1.540C	1.5636	1.5814	1.5881	1.6251	1.6432	1.6818	1.6913	1.7097
1.5091	1.5252	1.5492	1.5665	1.5918	1.6088	1.7C29	1.6534	1.67C0	1.7048

R-centroids (File: RCENTROID.DAT)

4	3
0.	.769602
1218.7	-.0063
-7.28	0.
30294.9	.5562
797.31	-.0048
-3.72	0.
221.5	.775156
1218.70	-.0063
-7.28	0.
30384.1	.6013
798.78	-.0046
-3.59	0.

Dunham Coefficients (File: DUNHAM.COF)

7
 .313 .110 .100 .06 .0424 .0000625 .000003
 .188 .066 .060 .0360 .0254 .000037506 .000002

Vibrational Population Weights (File: POPLTN.WT)

F30030
 32030
 34030
 36030
 38030
 40030
 42030
 44030
 46030
 48030
 50030
 52030

List of Experimental OMA Files (File: FILE.OMA)

4000.000	4200.000	1.000000	1200.000	450.0000
S(B->X) SPECTRUM AT 3 TORR				
0	1	200.0000	0.000000E+00	0.000000E+00
1.000000	1			

Input File Generated by Code (File: INPUT.DAT)

NS(B) SPECTRUM AT .74 TORR

ROT TEMP- 1.4000x10³
 -- SYNTHETIC SPECTRUM
 - EXPR. SPECTRUM
 V 1/2-1/2POP 3/2-3/2POP
 0 2.52x10⁻¹ 1.52x10⁻¹
 1 1.28x10⁻¹ 7.70x10⁻²
 2 1.39x10⁻¹ 8.30x10⁻²
 3 8.20x10⁻² 4.90x10⁻²
 4 2.10x10⁻² 1.25x10⁻²
 5 9.00x10⁻⁴ 5.00x10⁻⁴
 6 9.00x10⁻⁴ 5.00x10⁻⁴

(1,9)1/2
 (0,8)1/2
 (0,8)1/2
 (2,9)1/2
 (1,8)1/2
 (0,7)1/2
 (0,7)1/2
 (1,7)1/2
 (0,8)1/2
 (3,6)1/2
 (2,6)1/2
 (0,4)1/2
 (2,5)1/2
 (1,4)1/2
 (0,5)1/2
 (1,3)1/2
 (0,4)1/2
 (2,3)1/2
 (1,2)1/2
 (0,1)1/2
 (2,2)1/2
 (1,1)1/2
 (0,0)1/2
 (2,1)1/2
 (1,0)1/2
 (3,1)1/2
 (2,0)1/2
 (4,1)1/2
 (3,0)1/2
 (4,0)1/2

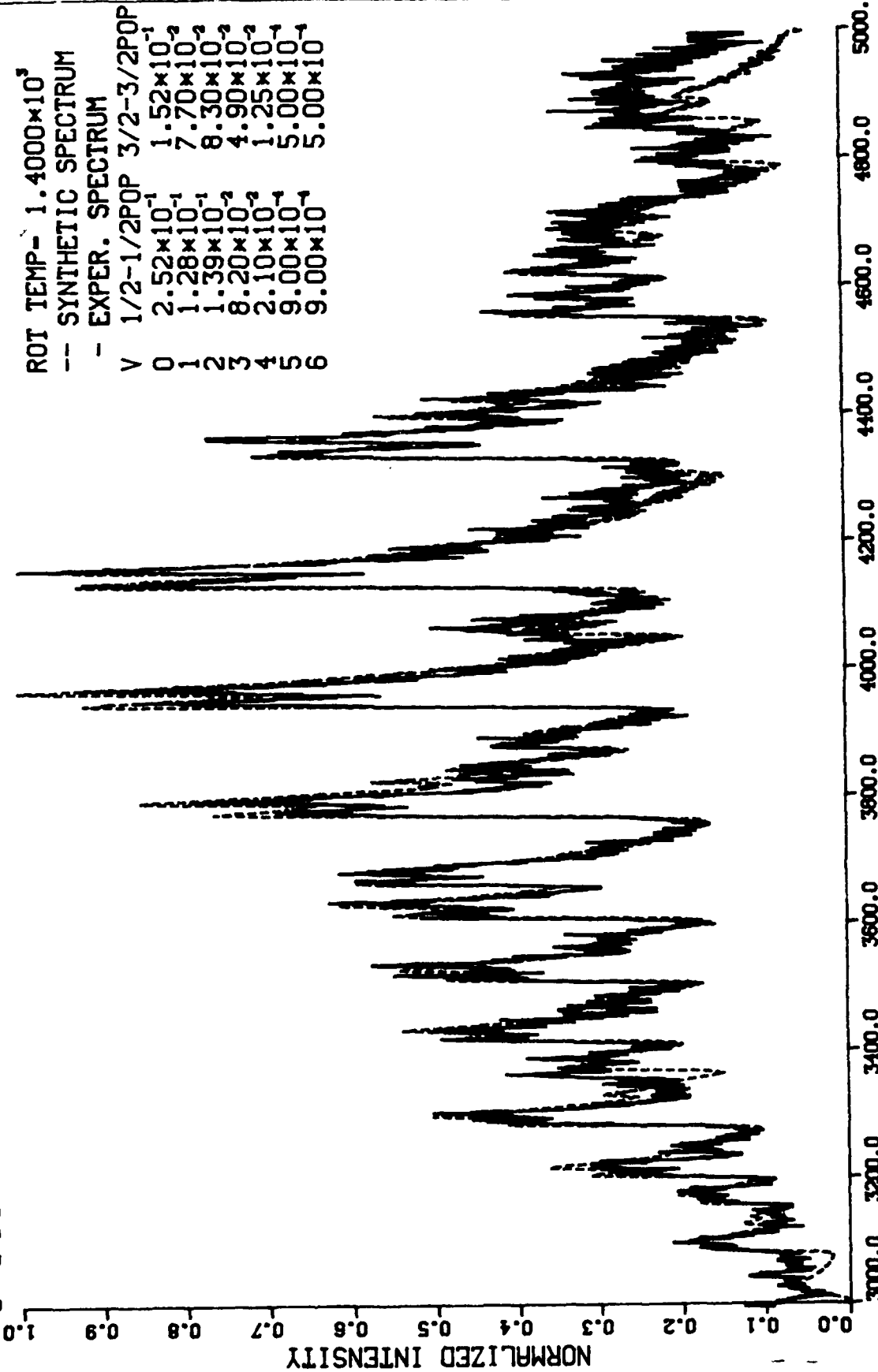


FIGURE 2

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