Simulation of Infrared Spectra

C. H. DOUGLASS, AND R. T. LODA

Applied Research Corporation
Landover, MD 20785

H. H. NELSON

Chemistry Dynamic and Diagnostic Branch
Chemistry Division

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**Simulation of Infrared Spectra**

Programs have been developed to simulate absorption and emission spectra of atmospheric and combustion product species. The programs use tabulated constants of the molecules of interest to calculate transition frequencies and line strengths as a function of temperature. Asymmetric rotors and linear molecules have been included. The calculated emission and absorption spectra can be compared to experimental spectra and can be used to predict spectral shifts due to isotopic substitution. Results for a variety of materials and conditions are presented.
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SIMULATION OF INFRARED SPECTRA

INTRODUCTION

The Naval Research Laboratory supports a number of programs concerning the infrared (IR) spectral characteristics of the materials produced by the combustion of a variety of types of fuels. These programs include measurements of the IR absorption and emission spectra of the combustion plumes of various materials under differing conditions. In an effort to more fully understand the combustion processes, a spectral simulation effort has been initiated. The purpose of this effort is to develop the capability of simulating IR spectra for comparison with experimental results. The molecules of interest in the simulation effort are atmospheric constituents and their isotopic variants.

Programs have been developed to simulate the absorption and emission spectra of these materials at different temperatures and under varying conditions. This report discusses the structure of the programs and the input data which are required. Results of calculations for a variety of materials and conditions are also presented.

PROGRAM STRUCTURE

Programs have been developed to calculate the spectra of isotopic variants of water (H₂O, HDO, and D₂O), CO₂, and HC and DCl. All programs are written in FORTRAN and run on the IBM AT computer. In the sections below, the theoretical underpinning of each set of programs is discussed. A general discussion of the program structure follows and then the details of program implementation are outlined. Copies of the program codes are included in the Appendix. Also in the Appendix are sample parameter files showing the structure and formatting of the input files. For both water and CO₂, actual input and output files are included. The discussion for each molecule assumes that an absorption spectrum is to be calculated. The changes in the program necessary to calculate an emission spectrum are detailed.

Calculations For Isotopic H₂O

The most difficult calculation is that for water which is an asymmetric rotor. King, Hainer and Cross originally determined expressions for the energy levels of an asymmetric rotor [1]. Each energy level is characterized by J, the total angular
momentum, and by two pseudo-quantum numbers, $K_{-1}$ and $K_1$. The pseudo-quantum numbers are used to distinguish between the $2J+1$ levels that have the same value of $J$. A level is labelled by the values of $K$ to which it corresponds in the prolate symmetric rotor ($K_{-1}$) and in the oblate symmetric rotor ($K_1$). These two values are combined to define an asymmetry parameter $r$

$$r = K_{-1} - K_1$$

The parameter $r$ assumes the values $-J, -J+1, ..., 0, ..., J-1, J$. The energy levels are ranked in order by the value of $r$ with the lowest energy level for a given $J$ being that with $r = -J$ and the highest that with $r = J$. In addition, $r$ serves as an index to the parity of the levels. For molecules belonging to the $C_{2v}$ point group, those levels with even $|r|$ are symmetric with respect to interchange of identical nuclei and those with odd $|r|$ are antisymmetric with respect to interchange of identical nuclei.

Cross, Hainer, and King also derived a means of calculating line strengths for the lines in an asymmetric rotor spectrum [2]. The line strength calculation requires the evaluation of the matrix elements of the direction cosines which are the elements of an orthogonal transformation from molecule-fixed to space-fixed coordinates. Application of their method allows calculation of the line strength of a particular transition as a function of the asymmetry of the rotor.

The starting point for the programs described herein was a program coded by Y. Endo and kindly provided by J.E. Butler (Code 6170, Chemistry Division, Naval Research Laboratory, Washington, D.C.). The program was designed for analysis of microwave spectra of asymmetric rotors. The calculation of the transition frequencies was not altered, but the intensity calculation required considerable modification (e.g., in the original program the temperature could not be varied). The dependence of the line intensity $S$ for an absorption at the frequency $\nu$ is given by the following expression (note that, since only relative intensities from the calculation are used, proportionalities
may be used instead of equalities:

$$S \propto \left( \frac{\nu_o}{v_0} \right) \left[ 1 - \exp(-c_2 \nu_o T_o) \right] g F Q_R(T_o) \exp(-c_2 E_R^{-} T_o) \ell^2 S_v^0(T_o)$$  \hspace{1cm} (1)

\( \nu_o \) = band center

\( c_2 \) = second radiation constant

\( T_o = \text{reference temperature} = 296 \text{K} \)

\( g \) = statistical weight of lower state

\( F \) = vibration - rotation interaction constant

\( Q_R(T_o) \) = rotational partition function at \( T_o \)

\( E_R^{-} \) = rotational energy of lower state

\( \ell^2 \) = direction cosines matrix element connecting lower and upper states

\( S_v^0(T_o) \) = band strength at \( T_o \)

The band strength depends on the following factors:

$$S_v^0 \propto \frac{\nu_o |R|^2}{Q_v(T_o)} \exp \left( -c_2 G_v^{-}/T_o \right)$$  \hspace{1cm} (2)

\( R \) = matrix element of the rotationless electric dipole moment

\( G_v^{-} \) = vibrational energy of lower state

\( Q_v(T_o) \) = vibrational partition function at \( T_o \)

Some comment is necessary on several of the terms included above. The term in square brackets in equation (1) is the induced emission term. It is negligibly small for the case in which \( c_2 \nu_o \gg T \) but is included for completeness. The statistical weight or nuclear statistics factor \( g \) depends on the symmetry of the lower state and will be discussed further below. The vibration-rotation interaction factor will be assumed to be equal to one in most cases. The band strength for the vibrational transition is available from tabulated values.

The temperature dependence of the line strength arises through the rotational and vibrational Boltzmann factors and the rotational and vibrational partition functions, as well as a small effect from the induced emission term. McClatchey [5] gives the temperature dependence as:
The temperature dependence for the bands in the water molecule can be written in somewhat simpler terms for two reasons: (1) the partition functions at T₀ are constants and can be omitted since only relative strengths are being calculated; and (2) the vibrational Boltzmann factor is equal to one because all bands considered have the vibrational ground state as the lower state. Note that the temperature dependence of the induced emission term can be accounted for by multiplying by the ratio of that term at temperature T to that at temperature T₀, cancelling out the T₀ term. The resulting expression for the line intensity at a temperature T is

\[ S \propto \nu \left\{ 1 - \exp\left(-c_\nu (T)/T_0\right) \right\} \exp\left(-c_\nu S_\nu(T_0)/T\right) \]

The program which calculates spectra for isotopic water reads input data from a parameter file. This file identifies the molecule for which the spectrum is to be calculated and supplies the information necessary for the simulation; for a complete description of the parameter file, see below. The program calculates the transition frequencies and the line intensities. All lines with frequencies within the specified range and intensities greater than the chosen minimum are stored. After all lines have been calculated, the stored lines are sorted in order of increasing frequency. The lines are then grouped into bins of equal width with the summed intensity of all lines within the bin at the center of the bin. A Gaussian lineshape is applied to the intensity to adjust the resolution for comparison with experimental spectra. An output file is then written for plotting the spectrum.

The parameter file contains the necessary inputs for the calculation. The parameters are discussed here in the order in which they appear in the parameter file.
See pages A2 and A3 for sample parameter and input files. ISOTOPE identifies the particular isotope under consideration: 161 for H₂O, 262 for D₂O, and 162 for HDO. The upper and lower state rotational constants and centrifugal distortion constants are read into the array PAR(I). NBINS is the number of bins of equal width into which the frequency range is divided. WIDTH is the halfwidth of the Gaussian lineshape which is applied. The variable IITY codes the band type of the vibrational transition - 100 for type A transitions, 010 for type B transitions, and 001 for type C transitions. The minimum and maximum values of J are JMIN and JMAX. The maximum change allowed in J is KTAU. The allowed frequency range is determined by the minimum and maximum frequency values FMIN and FMAX. The band center of the vibrational transition is FNUZ. STMIN is the minimum strength requirement for transitions to be stored. The temperature for the simulation is TT and the band strength for the transition is BS. The fundamental vibrational frequencies of the molecule are FNUU, FNU2, and FNU3. After the data have all been read in, they are printed to the screen so that it may be verified that the values are correct.

The program calculates frequencies and intensities for each branch in turn with the R branch first, followed by the P branch and then the Q branch. Once calculated, the frequency is tested to determine whether it falls between the limits of the frequency range. If so, a level name is determined and the strength is calculated. The strength calculation is divided into a number of steps. The direction cosines matrix element is calculated and multiplied by the rotational Boltzmann factor divided by the rotational partition function. The energy used in the Boltzmann factor is the initial state rotational energy ELI. The result of this calculation is multiplied by the nuclear statistics factor to give the parameter STRENGTH. The value of the statistical weight factor is determined by symmetry of the levels under interchange of identical nuclei and is indexed by the oddness or evenness of J. Table I gives the statistical weight factors for the isotopes of water. As STRENGTH for each level is determined, the values are summed to give TOTINT. To compare intensities correctly for different isotopes, the
intensities must be normalized by TOTINT. This is accomplished by dividing the strength of each line by TOTINT in the SORT subroutine. The calculation of the line intensity is completed by multiplying STRENGTH by the frequency, the induced emission term and the band strength, then dividing by the frequency of the band center and the vibrational partition function. Note that dividing by the band center is required because the band center is included in the tabulated $S^0_v(T_0)$ value.

After the line intensity is calculated, that value is compared to STMIN; if it exceeds the minimum strength criterion, the frequency, strength, and level name are stored. This process is continued until all lines in all three branches have been calculated. The line counter NLINE is incremented each time a line is stored. After all lines have been calculated, the lines are arranged in order of increasing frequency by the SORT subroutine. The SORT subroutine also performs the normalization by TOTINT described above. Because this normalization occurs after the comparison of the calculated line intensity to STMIN, the minimum strength value in the lines listed in the program output may not correspond directly to STMIN. The PRINT subroutine then prints out information for each stored line: the band type; the branch; the final and initial values of $J$, $K_z$, and $K_\ell$; the transition frequency; the calculated strength; and the relative strength calculated by dividing each line strength by the maximum line strength.

Next the subroutine BINSORT sorts all lines into bins of equal width, that width being $(FMAX-FMIN)/NBINS$. The SHAPE subroutine applies a Gaussian lineshape of half-width WIDTH to the summed intensity at the center of each bin. The total intensity of each bin is calculated as SMOOTH(I) after application of the lineshape. The SHAPE subroutine also writes an output file containing FMIN, FMAX, NBINS, and SMOOTH(I), I=1 to NBINS.

The program described above must be modified to calculate an emission spectrum rather than an absorption spectrum. There is of course no change in the transition frequencies. The population of the emitting species is that of the upper state rather than the lower state. The energy used in the rotational Boltzmann factor is now the
final state rotational energy ELF rather than ELI (i.e., terminology of the absorption process is retained; "final state" actually refers to the upper state). Since the molecule must also be in the excited vibrational state to emit, a vibrational Boltzmann factor $\exp(-e^*FNUZ \cdot \text{TT})$ must be used. The induced emission term is not used for the emission calculation. The index for the statistical weight factor is applied to the upper state rather than the lower state. In emission, a factor of $\nu^4$ rather than $\nu$ is used in the intensity calculation [5]. With the exception of these modifications, the program for emission is the same as that for absorption.

Calculations For CO$_2$

The calculation for a linear molecule is considerably simpler than that for an asymmetric rotor since expressions for the energy and the intensity can be expressed in closed form. The expression for the energy [6] is

$$E(J) = BJ(J+1) - DJ^2(J+1)^2 + HJ^3(J+1)^3$$

Values of the constants are given in the literature. For $\Sigma$ states, the calculation is straightforward. In calculating energies for $\Pi$ states, the effect of $\ell$-type doubling must be considered [6]. Separate constants are tabulated for $\varepsilon$ and $\delta$ sublevels of $\Pi$ states so both manifolds may be calculated.

In analyzing a particular transition, attention must be paid both to which levels are populated and to the selection rules governing the transition. $\Sigma^+_{u} - \Sigma^+_{g}$ transitions are straightforward because the $\ell$-type doubling is absent; only P and R branches appear. For $\Pi_u - \Sigma^+_{g}$ transitions, a Q-branch appears in addition to the P and R branches. For molecules such as CO$_2$ with the spins of the nuclei equal to zero, only the symmetric levels with respect to interchange of equivalent nuclei are occupied. The selection rules require the combination of symmetric with symmetric levels. The occupied levels in the $\Sigma$ state are those with even $J$ and the absorptions terminate in the $\varepsilon$ sublevels of the upper state levels with odd $J$ for the P and R branches. The Q branch transitions terminate in the (symmetric) $\delta$ sublevels of the upper state levels with even $J$. For a $\Pi_4 - \Pi_u$ transition, P, Q, and R branches are allowed. The symmetric levels for a $\Pi$ state
are e sublevels with odd J, f sublevels with even J. Thus two sets of P and R branches arise - an e-e set with odd J in the lower state and an f-f set with even J in the lower state. Since the Q branch transitions must connect two symmetric levels, the e <-> f selection rule is followed. The Q transitions with odd J originate in e sublevels and terminate in f sublevels. The Q transitions with even J originate in f sublevels and terminate in e sublevels.

The expression for the intensity calculation for CO₂ bands is given explicitly by Rothman [7].

\[ S = \nu S_0^0 S_{J\ell} \exp \left(-c_2 E_R T_o \right) \left[1-\exp(-c_2 \nu T_o)\right] \frac{E}{Q_R(T_o)} \]  

where \[ S_0^0 = \frac{8\pi^3 g I_3}{3hc Q_o(T_o)} \nu \nu_{3\ell} \exp \left(-c_2 G_v T_o \right) \] 

All terms are as defined previously; \( S_{J\ell} \) is the Hönig-London factor and \( I_3 \) is the isotopic abundance. We will consider only the isotope containing \(^{12}\)C and \(^{16}\)O; the constants will be dropped since only relative values are of importance. The temperature dependence is introduced in the same manner described above for H₂O. One complication in the CO₂ case is the fact that the lower state is not the ground vibrational state in all cases. That means that the vibrational Boltzmann factor which is included in the band strength may not be equal to one. In changing temperatures, it is necessary to divide by \( \exp(-c_2 G_v T_o) \) and to multiply by \( \exp(-c_2 G_v T_o) \) to calculate correctly the population in the lower state at a temperature \( T \).

The initial section of the program reads input data from a parameter file. The parameters are discussed here in the order in which they appear in the parameter file. See pages A40 and A41 for sample parameter and input files. The first parameter read is ID which identifies the type of band to be calculated: ID=11 for a \( \Sigma_u^- \Sigma_u^- \) band; ID=22 for a \( \Pi_g \Sigma_u^- \) band; ID=25 for a \( \Pi_u \Pi_u \) band. If ID=11, only P and R branches are calculated; if ID=22 or ID=25, P, Q, and R branches are calculated. The next set of parameters contains the upper state constants +BU, DU, and Hu to be used for the
calculation of energy levels. For the $\Pi_u^+ - \Sigma^+_u$ transition, the upper state energy levels are those for the $e$ sublevel for the P and R branches. For the $\Pi_u - \Pi_u$ transition, two separate parameter files must be used for P and R branches - one using the $e$ sublevels for odd $J$ and one using the $f$ sublevels for even $J$. The next parameters read are B, DUQ, and HUQ, the upper state levels used to calculate Q branch transitions. For the $\Pi_u^+ - \Sigma^+_u$ transition, these are for the upper state $f$ sublevels. For each of the $e-e$ and $f-f$ pairs for the $\Pi_u^- - \Pi_u^+$ transition, the alternate set of sublevels is used for the $Q$ branch upper state since the $e <-> f$ selection rule is followed. The final set of parameters BL, DL, and HL is used for the calculation of the lower state energy levels. The next set of entries in the parameter file gives minimum and maximum values of $J$ (JMIN and JMAX) and of the frequency (FMIN and FMAX). Note that in the energy level and transition frequency calculations, $J$ is incremented by 2. The minimum value of $J$ thus determines whether the $J$ values will be odd or even. The following three frequencies FNU1, FNU2, and FNU3 are the fundamental frequencies of the molecule. The next line gives the band center frequency (FNUZ) and the vibrational energies of the lower (FLOW) and upper (FHIGH) states involved in the transition. Next the band strength SV and temperature TT are input. For the $\Pi_u^- - \Pi_u^+$ transition, the band strength is equally split between the $e-e$ and $f-f$ pairs. The final line in the parameter file contains NBINS and WIDTH.

Following printing of the input data to the screen, three sets of energy levels are calculated for the indicated range of $J$: EU(1), the upper state levels; EL(1), the lower state levels; and EUQ(1), the upper state levels of the other sublevel set for calculation of the $Q$ branch transitions. Changes in rotational energies for P and R branches (EROTP and EROTR) are calculated; for transitions involving a $\Pi$ state, the changes in rotational energy for the $Q$ branch (EROTQ) are also calculated. The vibrational Boltzmann factor and the rotational and vibrational partition functions are calculated at $T_1$ and at $T$. For the absorption calculation, the vibrational Boltzmann factor uses FLOW. In a series of loops, the frequencies and intensities of the individual lines in
each branch are calculated. One of the factors in the strength calculation is the Hönli-London factor. The Hönli-London factor depends on both \( \Delta J \) and \( \Delta \ell \). The values for the bands of \( \text{CO}_2 \) which are considered are given in Table 2 with \( J \) representing the lower state quantum number. If the frequency of the transition is within the frequency range from \( \text{FMIN} \) to \( \text{FMAX} \), the frequency, strength, and line label are stored. The \text{SORT}, \text{PRINT}, \text{BINSORT}, \text{and SHAPE} subroutines are analogous to those described above for the water calculation.

The transformation from absorption to emission requires the same sort of changes as in the water case. The induced emission term is not used. The vibrational and rotational Boltzmann factors use upper state energy levels rather than lower state energy levels. In the intensity calculation, \( \nu^4 \) replaces \( \nu \). The remainder of the calculation is identical to that for absorption.

\textbf{Calculations for HCl and DC\textsubscript{3}}

The calculations for the diatomics HCl and DC\textsubscript{3} are straightforward and will not be described in detail here. Only the \( ^{35}\text{Cl} \) isotope was included and only emission spectra were calculated.

\textbf{Program Listings}

Copies of all the programs used are included in the Appendix. The executable file \texttt{ASYMABS} was used for absorption calculations for the water isotopes. It was formed by linking \texttt{ASYMABS + ASYMSUB + SHAPE + BINSORT}. The emission calculations for water used \texttt{ASYMEMS}, forming by linking \texttt{ASYMEMS + ASYMSUB + SHAPE + BINSORT}. The corresponding absorption (emission) program for \( \text{CO}_2 \) was \texttt{CO2ABS (CO2EMS)}, formed by linking \texttt{CO2ABS (CO2EMS) + CO2SUB + CO2SHAPE + CO2BSORT}. The HCl program linked HCLEMS + HCLSUB + HCLSHAPE + HCLBSORT.

The Appendix also includes Sample Parameter Files for H\textsubscript{2}O and \text{CO}_2 showing the structure of the input data files and the formats used for the variables. In addition, there are actual examples of input data files H\textsubscript{2}ONU'1 and CO2NU'3 used for the \( \nu_3 \) band of H\textsubscript{2}O and the \( \nu_3 \) band of \text{CO}_2. The sample output files generated by running
ASYMABS and CO2ABS respectively are also shown. These may be useful as tests in trying to implement the programs.

RESULTS AND DISCUSSION

The input parameters for the three isotopes of water were collected from a variety of sources, since no one reference was identified in which a complete set for the bands under consideration was compiled. The region of the spectrum selected for consideration was 0 - 5000 cm\(^{-1}\). The bands that make a significant contribution in this region can be identified from the AFGL band strength listing. The most recent version for the H\(_2\)O bands was the 1980 update [8]. The four bands with a band strength greater than 0.5% of the largest were used in the calculation. These are the three fundamentals and the first overtone of the bending mode. The \(\nu_2 + \nu_3\) combination band has significant intensity and is centered at 5331 cm\(^{-1}\). Although the lower frequency edge extends beyond 5000 cm\(^{-1}\), this band was not found to make a significant contribution. The pure rotational spectrum was not included.

The rotational and vibrational parameters used for the H\(_2\)O calculations are given in Table 3. For the H\(_2\)O calculations, centrifugal distortion constants are included for all bands. The corresponding parameters for D\(_2\)O are given in Table 4. but centrifugal distortion constants are not included. Note that the band strengths are from a calculation by Wilemski [14] because experimental values could not be found. The \(2\nu_2\) band is omitted because no band strength could be found; by analogy to H\(_2\)O and HDO, it would make a small contribution at most. Table 5 contains the constants for HDO. Note that each band has both A and B type character; separate band strengths are given for each contribution.

The results of calculations for absorption by H\(_2\)O at 296K, 1000K, and 1730K are shown in Fig. 1. The intensity is given in arbitrary units; the intensities of the absorption spectra at different temperatures are correctly scaled relative to each other. The width parameter here is 2 cm\(^{-1}\). corresponding to a resolution of 4 cm\(^{-1}\). The lowest frequency band at 1594 cm\(^{-1}\) is the \(\nu_3\) bending mode. The very small
contribution from $2\nu_2$ lies at 3155 cm$^{-1}$; it can be seen in 296K spectrum. The $\nu_1$ and $\nu_2$ bands overlie one another in the 3500-4000 cm$^{-1}$ region. As the temperature increases, the spectra broaden as higher $J$ levels are populated and absorb. The intensity of the absorption decreases as the temperature increases because of the decrease in population of the absorbing state. To determine the accuracy of the calculated spectra, the frequencies of lines in the calculated spectra were compared to tabulated values for each of the bands studied. The calculated values agreed with literature values to within 1 cm$^{-1}$ in most cases with some deviations of 3-4 cm$^{-1}$ observed. The results were not as good for individual line strengths. Variations of 50% or more were noted in comparing calculated and literature values. The purpose of this study, however, was to determine the region in which emission occurs rather than the line-by-line strength of particular portions of the spectrum. The accuracy achieved is certainly adequate for that purpose.

Emission spectra at 1730K are shown for all three isotopes in Fig. 2. The substitution of one D for H in water shifts $\nu_1$ from 3657 cm$^{-1}$ to 2724 cm$^{-1}$, giving three distinct bands. In going to D$_2$O, once again $\nu_1$ and $\nu_3$ are in the same region but all bands are shifted to lower frequency. Again all spectra are scaled correctly relative to each other and correspond to a resolution of 4 cm$^{-1}$. It is clear from Fig. 2 that changing from H$_2$O to D$_2$O shifts the most intense absorption band into a significantly different region of the spectrum. Fig. 3 shows a composite emission spectrum at 1730K for an equimolar mixture of H$_2$O and D$_2$O.

Table 6 gives the rotational and vibrational constants for CO$_2$. The bands included are those five for which $S^0>10^{24}$ cm/molecule. Three of these are $\Sigma-\Sigma$ transitions with one $\Pi-\Sigma$ transition and one $\Pi-\Pi$ transition. The lower state for the $\Pi-\Pi$ transition is not the ground vibrational state but instead is the 01101 state (for band notation, see [3]). Absorption spectra calculated at 296K, 1000K, and 1730K are shown in Fig. 4, correctly scaled relative to one another. The most prominent band at 2349 cm$^{-1}$ is the $\nu_2$ fundamental. The $\nu_2$ fundamental appears at 667 cm$^{-1}$ and small contributions are made
by combination bands in the 3600-3700 cm\(^{-1}\) region. As the temperature is increased, the absorption decreases because of the smaller number of molecules in the lower vibrational state. The relative importance of the 2300 cm\(^{-1}\) peak increases relative to the 667 cm\(^{-1}\) peak because of the contribution made to the higher frequency peak by the \(\Pi-\Pi\) transition originating in the 01101 state. This excited lower state has a higher population at the higher temperature and the absorption due to this transition therefore is increased. Figure 5 shows emission due to CO\(_2\) at 1000K and 1730K with correct relative scaling. The 2300 cm\(^{-1}\) feature is again the predominant one with its importance relative to the 667 cm\(^{-1}\) band increasing with increasing temperature. The contribution due to the 3600-3700 cm\(^{-1}\) peaks is small even at 1730K. Figure 6 shows on an expanded scale the main CO\(_2\) band with emission calculated at 1730K and absorption calculated at 296K. The maximum value of each spectrum is individually scaled to a value of 10. If a material producing hot CO\(_2\) were burned and the spectrum observed through an atmospheric path, the cold CO\(_2\) in the atmosphere would absorb the radiation making up the central portion of the emission spectrum. The observed spectrum would show only the wings of the hot CO\(_2\) spectrum, as shown in the lower panel of Fig. 6.

Table 7 gives the rotational and vibrational constants used to calculate the HCl and DCI spectra. The calculation also used a vibration-rotation interaction constant expression [22]:

\[
F = 1 - 2.5599 \times 10^{-2} m + 3.203 \times 10^{-4} m^2
\]  

(8)

Emission spectra for HCl and DCI at 1730K are shown in Fig. 7. Again it is clear that deuteration of HCl shifts the emission into a different region of the spectrum.

**CONCLUSIONS**

Spectral simulation programs have been developed which correctly calculate the spectra of species produced in the combustion of a variety of fuels. The programs calculate both positions and intensities in the vibrational-rotational spectra of isotopic forms of H\(_2\)O, CO\(_2\), and HCl. The calculated values of the frequencies agree well with
tabulated values while the agreement of intensities with literature values is not as good.

As expected, the regions of emission and absorption shift markedly with isotopic substitution. The relative importance of particular transitions varies with temperature. The simulated spectra can be combined to mimic observation through an atmospheric path where both emission and absorption due to the same species are important.
References

APPENDIX

The Appendix contains program listings, sample inputs, and sample outputs for the programs described in the preceding report. Contents of the Appendix are listed below.

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PAR(7)  PAR(8)  PAR(9)
PAR(16) PAR(17) PAR(18)
PAR(19) PAR(20) PAR(21)
PAR(22) PAR(23) PAR(24)
NBINS[I5] WIDTH[F10.6]

ISOTOPE = isotope code
PAR(1), PAR(2), PAR(3) = A, B, C constants for upper state
PAR(4) - PAR(8) = distortion constants for upper state
PAR(16), PAR(17), PAR(18) = A, B, C constants for lower state
PAR(19) - PAR(23) = distortion constants for lower state
NBINS = number of bins
WIDTH = Gaussian halfwidth
ITY = band type
JMIN, JMAX = minimum and maximum values of J
KTAU = maximum change in TAU
FMIN, FMAX = minimum and maximum values of frequency
FNUZ = band center
STMIN = minimum strength
TT = temperature
BS = band strength
FNU1, FNU2, FNU3 = fundamental frequencies
SAMPLE INPUT FILE H2ONU1

```
161
27.12217  14.3047  9.1045
0.001233  -0.0053874  0.03023
0.00049987  0.0012405  0.0
27.880678  14.521689  9.277459
0.00124894  -0.0057655  0.0325199
0.00050838  0.0013007  0.0
5000  2.0
010  0  25  5
0000.  5000.  3657.053
1.50  296.  48.62
3657.053  1594.778  3755.93
```
PARAMETER FILE = H2ONU1

OUTPUT FILE = H2OANU1

ISOTOPE = 161

UPPER STATE CONSTANTS
A = 27.1222  B = 14.3047  C = 9.1045
DLJ = 0.00123300  DLJK = -0.00538740  DLK = 0.03023000
DSJ = 0.00049987  DSK = 0.00124050

LOWER STATE CONSTANTS
A = 27.8807  B = 14.5217  C = 9.2775
DLJ = 0.00124894  DLJK = -0.00576550  DLK = 0.03251990
DSJ = 0.00050838  DSK = 0.00130070

SELECTION RULES
J RANGE 0 TO 25

MAX. DELTA TAU 5
FREQ. RANGE 0.0000 TO 5000.0000 CM⁻¹
BAND ORIGIN 3657.0530 CM⁻¹
NU #1 3657.0530 CM⁻¹
NU #2 1594.7780 CM⁻¹
NU #3 3755.9300 CM⁻¹
MIN. STRENGTH 1.500000
TEMPERATURE 296.00
NBINS 5000
WIDTH 2.000000
TOTAL NUMBER OF LINES = 19

TOTAL BAND INTENSITY = 7.5561E-01

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TOTAL BAND INTENSITY (GAUSSIAN SUM) = 4.9228E+01

MAXIMUM INTENSITY = 1.3810E+00
PROGRAM ASYMABS.FOR
IMPLICIT REAL*8(A-H,O-Z)

ASYMMETRIC ROTOR FREQUENCY ESTIMATION PROGRAM FOR INFRARED AND VISIBLE SPECTROSCOPY Coded by Y.E.

MODIFIED BY C.H.D., R.T.L., H.H.N.

DIMENSION NAME(18),HD(50),HF(50),HDLO(50),HFL0(50),
EL(50),ELLO(50),CFAC(50),CFACP(50),TVF(50),
TVI(50),LTYPE(3),P(30)

LOGICAL LTYPE
COMMON /CON/ PAR(30)
COMMON /FREQ/ FMIN,FMAX
COMMON /BINS/ BINST(5000),BINDEX(5000),NBINS,WIDTH
COMMON /OUTPUT/ ACCESS$,ACCESS1$
CHARACTER*24 ACCESS$,ACCESS1$
CHARACTER*8 FILENM$,FILNM$
INTEGER*2 IYEAR,IMONTH,IDAY,IHOUR,IMINUTE
CALL GETTIM(IHOUR,IMINUTE)
CALL GETDAT(IYEAR,IMONTH,IDAY)

ENTER NAME OF PARAMETER FILE TO BE USED AS INPUT

WRITE (6,*) 'ENTER INPUT FILE NAME?'
READ 99,FILENM$
FORMAT(A8)

ENTER NAME OF FILE TO BE USED FOR STORAGE OF OUTPUT

WRITE (6,*) 'ENTER OUTPUT FILE NAME?'
READ 99,FILNM$

THE INPUT PARAMETER FILE IS LOCATED ON DRIVE C: IN SUBDIRECTORY ASYMRTR

THE OUTPUT FILE IS WRITTEN TO DRIVE A:

ACCESS$ = 'C:\ASYMRTR\\'//FILENM$//' .DAT'
ACCESS1$ = 'A:\'//FILNM$//' .DAT'
OPEN (2,FILE=ACCESS$,ACCESS='SEQUENTIAL')

ISOPTOPE CODE IS READ:
161 = H2O
162 = D2O
162 = HD0
READ(2,*) ISOTOPE

THE VARIABLES ARE READ FROM THE PARAMETER FILE:

- PAR(1,2,3) = A,B,C VALUES FOR THE UPPER STATE
- PAR(4,5,6,7,8) = CENTRIFUGAL DISTORTION CONSTANTS
  FOR THE UPPER STATE
- PAR(10-15) = UNUSED IN PRESENT VERSION; ALL = 0
- PAR(16,17,18) = A,B,C VALUES FOR THE LOWER STATE
- PAR(19,20,21,22,23) = CENTRIFUGAL DISTORTION
  CONSTANTS FOR THE LOWER STATE
- PAR(24-30) = UNUSED IN PRESENT VERSION; ALL = 0

DO 111 I=1,7,3
111 READ(2,*) (PAR(J), J=I,I+2)

DO 121 I=10,15
121 PAR(I)=0.
DO 131 I=16,22,3
131 READ(2,*) (PAR(J), J=I,I+2)
DO 141 I=25,30
141 PAR(I)=0.

READ NBINS = NUMBER OF BINS INTO WHICH FREQUENCY RANGE IS
DIVIDED AND WIDTH = HALF-WIDTH OF GAUSSIAN LINE SHAPE

READ (2,84) NBINS,WIDTH

READ IITY = BAND TYPE
  100 = A TYPE BAND
  010 = B TYPE BAND
  001 = C TYPE BAND

JMIN AND JMAX SET MINIMUM AND MAXIMUM VALUES OF J
KTAU = MAXIMUM CHANGE ALLOWED IN TAU

READ (2,69) IITY,JMIN,JMAX,KTAU

FMIN AND FMAX SET ALLOWED LIMITS FOR FREQUENCY RANGE
IN CM-1. FNUZ IS THE BAND CENTER IN CM-1

READ (2,79) FMIN,FMAX,FNUZ

STMIN = MINIMUM STRENGTH FOR STORAGE OF LINE
TT = TEMPERATURE
BS = BAND STRENGTH FOR TRANSITION BEING CALCULATED

READ(2,59) STMIN,TT,BS

FNU1,FNU2,FNU3 ARE THE FUNDAMENTAL FREQUENCIES IN CM-1

READ (2,79) FNU1,FNU2,FNU3
THE PARAMETERS READ FROM THE PARAMETER FILE ARE PRINTED OUT.

WRITE (6,6019)
6019 FORMAT (10X,'OUTPUT FROM PROGRAM ASYMABS.FOR///)
WRITE(6,6022) IMONTH,IDAY,IYEAR
6022 FORMAT(1X,I2,'/',I2,'/',I4)
WRITE(6,6023) IHOUR,IMINUTE
6023 FORMAT(1X,I2,'/',I2/) WRITE(6,6034) FILENM$
WRITE(6,6036) FILNM1$
WRITE(6,6029) ISOTOPE
6029 FORMAT(' ISOTOPE =',14//)
6034 FORMAT(' PARAMETER FILE = ',A8//)
6036 FORMAT(' OUTPUT FILE = ',A8//)
WRITE(6,6020) (PAR(I), I=1,8)
6020 FORMAT(' UPPER STATE CONSTANTS'//
1 ' A =',F16.5X,'B =',F16.5X,'C =',F16.4/
2 ' DLJ =',F16.5X,'DLJK=',F16.5X,'DLK =',F16.8/
3 ' DSJ =',F16.5X,'DSK =',F16.8//)
WRITE(6,6025) (PAR(I), I=16,23)
6025 FORMAT(' LOWER STATE CONSTANTS'//
1 ' A =',F16.5X,'B =',F16.5X,'C =',F16.4/
2 ' DLJ =',F16.5X,'DLJK=',F16.5X,'DLK =',F16.8/
3 ' DSJ =',F16.5X,'DSK =',F16.8//)
DO 100 I=1,3
100 LTYPE(I)=.FALSE.
IF (IITY.GE.100) LTYPE(1)=.TRUE.
IF (MOD(IITY,100).GE.10) LTYPE(2)=.TRUE.
IF (MOD(IITY,10) .GE. 1) LTYPE(3)=.TRUE.
WRITE(6,6030) LTYPE,JMIN,JMAX
6030 FORMAT(' SELECTION RULES ',3L4/
1 ' J RANGE ',I4,' TO ',I4)
WRITE(6,6040) KTAU,FMIN,FMAX,FNU1,FNU2,FNU3,
1 STMIN,TT,NBINS,WIDTH,BS
6040 FORMAT(' MAX. DELTA TAU ',I4/
1 ' FREQ. RANGE ',F10.4,' TO ',F10.4,' CM-1'
2 ' BAND ORIGIN ',F10.4,' CM-1'/
7 ' NU #1 ',F10.4,' CM-1'/
8 ' NU #2 ',F10.4,' CM-1'/
9 ' NU #3 ',F10.4,' CM-1'/
3 ' MIN. STRENGTH ',E12.3/
4 ' TEMPERATURE ',F7.2/
5 ' NBINS ',I5/
6 ' WIDTH ',F10.6/
7 ' BAND STRENGTH ',F10.4///)

SET LINE COUNTER TO ZERO
NLINE = 0

SET INITIAL TOTAL BAND INTENSITY = 0

TOTINT=0.0

DEFINE FCT = FACTOR FOR BOLTZMANN CALCULATIONS

FCT=-1.438786/TT

CALCULATE VIBRATIONAL PARTITION FUNCTION

VIBPF=1./((1.-DEXP(FCT*FNU1))*(1.-DEXP(FCT*FNU2))*(1.-DEXP(FCT*FNU3)))

CALCULATE ROTATIONAL PARTITION FUNCTION

ROTPF=(TT**3/(PAR(16)*PAR(17)*PAR(18)))**.5

DO 9000 J=JMIN,JMAX

PRINT J ON SCREEN TO TRACK PROGRESS OF CALCULATION

PRINT 6010,J

6010 FORMAT (1X,15)

C****** R BRANCH TRANSITIONS

IF (J.EQ.JMIN) GO TO 4000

FLJIN=1.DO/DBLE(J)

JLO = J-1

DO 2000 NTYPE=1,3

IF (.NOT.LTYPE(NTYPE)) GO TO 2000

DO 2100 ISYMF=1,4

ISYMI = ISEL(ISYMF,NTYPE,1)

CALL ECALC(0,ISYMF,J,HD,HF,EL,NHF,KMAXF,MXT)

CALL ECALC(1,ISYMI,JLO,HDLO,HFLO,ELLO,NHI,KMAXI,MXTLO)

IF (NHF*NHI.EQ.0) GO TO 2100

C****** CALCULATE DIRECTION COSINE

CALL CFACTR(1,NTYPE,NHF,NHI,KMAXF,KMAXI,J,CFAC,CFACP)

C****** RANGE OF ISHIFT

NTDEL = MXT-MXTLO

NSMAX = (KTAU-NTDEL+100)/4-25
NSMIN = 25-(KTAU+NTDEL+100)/4

DO 2200 ISHIFT=NSMIN,NSMAX
IF (ISHIFT.GE.0) GO TO 2180
N = MIN0(NHF+ISHIFT,NHI)
IF (N.LT.1) GO TO 2200
NPLUSF = -ISHIFT
NPLUSI = 0
GO TO 2210

2180 N = MIN0(NHF,NHI-ISHIFT)
IF (N.LT.1) GOTO 2200
NPLUSF = 0
NPLUSI = ISHIFT
2210 CONTINUE

C***** CALCULATE INDIVIDUAL TRANSITIONS

DO 2300 I=1,N
INOF = I+NPLUSF
INOI = I+NPLUSI
ELF = EL(INOF)
ELI = ELLO(INOI)
FREQ = (ELF-ELI)/1.+FNUZ

TEST WHETHER LINE POSITION IS WITHIN SPECIFIED
FREQUENCY RANGE. IF SO, CONTINUE WITH INTENSITY
CALCULATION; IF NOT, CALCULATE NEXT LINE.

IF (FREQ.GT.FMAX. OR. FREQ.LT.FMIN) GO TO 2300

C***** LEVEL NAMES

KAF = KMAXF+2*(1-INOF)
KCF = J+1-KAF-ISYMF+2*(ISYMF/2)
KAI = KMAXI+2*(1-INOF)
KCI = JLO+1-KAI-ISYMI+2*(ISYMI/2)

C***** CALCULATE EIGEN VECTORS

CALL EIVEC(NHF,HD,HF,ELF,TVF)
CALL EIVEC(NHI,HDLO,HFLO,ELI,TVI)

C***** CALCULATE LINE STRENGTH

FAC = 0.0DO
IPLUS = 0
IF (KMAXF-KMAXI.EQ.2) IPLUS = 1
NN = MIN0(NHF-IPLUS,NHI)
DO 2520 II=1,NN
2520 FAC = FAC+CFAC(II)*TVF(II+IPLUS)*TVI(II)
IF (NTYPE.EQ.1) GOTO 2540
FACP = 0.0D0
NN = MIN0(NHF-1,NHI)
IF (NN.LT.1) GO TO 2512
DO 2530 II=1,NN
2530 FACP = FACP+CFACP(II)*TVF(II+1)*TVI(II)
2512 IF (NTYPE.EQ.2) FACP = -FACP
FAC = FAC+FACP
2540 STRE = FAC**2*FLJIN

MULTIPLY DIRECTION COSINES FACTOR BY ROTATIONAL BOLTZMANN
FACTOR OVER ROTATIONAL PARTITION FUNCTION

STRE=(STRE*DEXP(-ELI/(0.695*TT)))/ROTPF

ASSIGN NUCLEAR STATISTICS FACTOR BASED ON IDENTITY OF
ISOTOPE AND WHETHER LEVEL IS ODD OR EVEN
H2O  1:3 FOR EVEN:ODD
D2O  6:3 FOR EVEN:ODD
HDO  1 FOR ALL LEVELS

KK=IABS(KAI-KCI)
IF(ISOTOPE.EQ.161) THEN
STNUC=(1.+2.*(REAL(MOD(KK,2))))
ELSEIF(ISOTOPE.EQ.262) THEN
STNUC=(6.-3.*(REAL(MOD(KK,2))))
ELSE
STNUC=1.0
ENDIF

STIMULATED EMISSION CONTRIBUTION IS CALCULATED.

STIMEM=(1.-DEXP(FCT*FREQ))

CALCULATE STRENGTH WHICH INCLUDES ROTATIONAL AND NUCLEAR
STATISTICS FACTORS. THIS WILL BE USED LATER TO NORMALIZE
FOR COMPARISON OF DIFFERENT ISOTOPES. TOTINT IS SUM OF
STRENGTH FOR EACH LINE.

STRENGTH=STNUC*STRE

CALCULATE FINAL INTENSITY BY MULTIPLYING BY THE INDUCED
EMISSION TERM, THE FREQUENCY, AND THE BAND STRENGTH AND
DIVIDING BY VIBRATIONAL PARTITION FUNCTION AND BAND CENTER.

STRE=(STRENGTH*STIMEM*FREQ*BS)/(FNUZ*VIBPF)

****** STORE THE CALCULATED TRANSITION IF STRE EXCEEDS THE
MINIMUM STRENGTH CRITERION.

IF (STRE.GE.STMIN) CALL STORE(NLINE,J,KAF,KCF,JLO,KAI,
1   KCI,FREQ,STRE,NTYPE)

2300 CONTINUE
2200 CONTINUE
2100 CONTINUE
2000 CONTINUE

C
C
C***** P BRANCH TRANSITIONS - P BRANCH TRANSITION FREQUENCIES
C AND STRENGTHS ARE CALCULATED BY THE SAME METHOD USED
C ABOVE FOR THE R BRANCH TRANSITIONS.
C
4000 CONTINUE

C
C IF (J.EQ.JMIN) GO TO 4200
FLJIN = 1.DO/DBLE(J)
JLO = J-1
C
C DO 3000 NTYPE=1,3
IF (.NOT.LTYPE(NTYPE)) GO TO 3000
C
DO 3100 ISYMF=1,4
ISYMI = ISEL(ISYMF,NTYPE,1)
CALL ECALC(1, ISYMF,J,HD,HF,EL,NHF,KMAXF,MAXT)
CALL ECALC(0, ISYMI,JLO,HDLO,HFLO,ELLO,NHI,KMAXI,MXTLO)
IF (NHF*NHI.EQ.0) GO TO 3100
C
C***** CALCULATE DIRECTION COSINES
C
CALL CFACTR(1,NTYPE,NHF,NHI,KMAXF,KMAXI,J,CFAC,CFACP)
C
C***** RANGE OF ISHIFT
C
NTDEL = MAXT-MXTLO
NSMAX = (KTAU-NTDEL+100)/4-25
NSMIN = 25-(KTAU+NTDEL+100)/4
C
C DO 3200 ISHIFT=NSMIN,NSMAX
IF (ISHIFT.GE.0) GO TO 3180
N = MIN0(NHF+ISHIFT,NHI)
IF (N.LT.1) GOTO 3200
NPLUSF = -ISHIFT
NPLUSI = 0
GOTO 3210
C
3180 N = MIN0(NHF,NHI-ISHIFT)
IF (N.LT.1) GOTO 3200
NPLUSF = 0
NPLUSI = ISHIFT
3210 CONTINUE
C
C***** CALCULATE INDIVIDUAL TRANSITIONS
C
DO 3300 I=1,N
INOFL = I+NPLUSF
INOI = I+NPLUSI
ELF = ELO\(\text{INOFL}\)
ELO = ELO\(\text{INOI}\)
FREQ = \(\text{ELI}-\text{ELF}\)/1.+FNUZ
IF (FREQ.GT.FMAX.OR.FREQ.LT.FMIN) GO TO 3300
C
C****** LEVEL NAMES
C
KAF = KMAXF+2*(1-INOFL)
KCF = J+1-KAF-ISYMF+2*(ISYMF/2)
KAI = KMAXI+2*(1-INOI)
KCI = JLO+1-KAI-ISYMI+2*(ISYMI/2)
C
C****** CALCULATE EIGEN VECTORS
C
CALL EIVEC(NHF,HD,HF,ELF,TVF)
CALL EIVEC(NHI,HDLO,HFLO,ELI,TVI)
C
C****** CALCULATE LINE STRENGTH
C
FAC = 0.0DO
IPLUS = 0
IF (KMAXF-KMAXI.EQ.2) IPLUS = 1
NN = MINO(NHF-IPLUS,NHI)
DO 3520 II=1,NN
3520 FAC = FAC+CFAC(II)*TVF(II+IPLUS)*TVI(II)
GOTO 3540
FACP = 0.0DO
NN = MINO(NHF-1,NHI)
IF (NN.LT.1) GO TO 3512
DO 3530 II=1,NN
3530 FACP = FACP+CFACP(II)*TVF(II+1)*TVI(II)
3512 IF (NTYPE.EQ.2) FACP = -FACP
FAC = FAC+FACP
3540 STRE = FAC**2*FLJIN
STRE=(STRE*DEXP(-ELI/(0.695*TT)))/ROTPF
KK=IABS(KAI-KCI)
IF(ISOTOPE.EQ.161) THEN
STNUC=(1.+2.*(REAL(MOD(KK,2))))
ELSEIF(ISOTOPE.EQ.262) THEN
STNUC=(6.-3.*(REAL(MOD(KK,2))))
ELSE
STNUC=1.0
ENDIF
STIMEM=(1.-DEXP(FCT*FREQ))
STRENGTH=STNUC*STRE
STRE=(STRENGTH*STIMEM*FREQ*BS)/(FNUZ*VIBPF)
C
C****** STORE THE CALCULATED TRANSITION
C
IF (STRE.GE.STMIN) CALL STORE(NLINE,JLO,KAI,KCI,J,KAF,
KCF,FREQ,STRE,NTYPE)
C 3300 CONTINUE
3200 CONTINUE
3100 CONTINUE
3000 CONTINUE
C
C 4100 CONTINUE
C
C***** Q BRANCH TRANSITIONS - Q BRANCH TRANSITION FREQUENCIES
C AND LINE STRENGTHS ARE CALCULATED BY THE SAME METHOD
C USED ABOVE FOR THE P AND R BRANCHES.
C
IF (J.EQ.0) GO TO 4200
FLJIN = DBLE(J+J+1)/DBLE(J*(J+1))
C
DO 7000 NTYPE=1,3
IF (.NOT.LTYPE(NTYPE)) GO TO 7000
C
DO 7100 ISYMF=1,4
ISYMI = ISEL(ISYMF,NTYPE,0)
CALL ECALC(0,ISYMF,J,HD,HF,EL,NHF,KMAXF,MXT)
CALL ECALC(1,ISYMI,J,HDLO,HFLO,ELLO,NHI,KMAXI,MXTLO)
IF (NHF*NHI.EQ.0) GO TO 7100
C
C*****CALCULATE DIRECTION COSINES
C
CALL CFACTR(0,NTYPE,NHF,NHI,KMAXF,KMAXI,J,CFAC,CFACP)
C
C***** RANGE OF ISHIFT
C
NTDEL = MXT-MXTLO
NSMAX = (KTAU-NTDEL+100)/4-25
NSMIN = 25-(KTAU+NTDEL+100)/4
C
DO 7200 ISHIFT=NSMIN,NSMAX
C
IF (ISHIFT.GE.0) GO TO 7320
N = MINO(NHF+ISHIFT,NHI)
IF (N.LT.1) GO TO 7200
NPLUSF = -ISHIFT
NPLUSI = 0
GO TO 7330
C
7320 N = MINO(NHF,NHI-ISHIFT)
IF (N.LT.1) GO TO 7200
NPLUSF = 0
NPLUSI = ISHIFT
C
C****** INDIVIDUAL TRANSITIONS
C
7300 DO 7300 I=1,N
INOF = I+NPLUSF
INOI = I+NPLUSI
ELF = EL(INOF)
ELI = ELLO(INOI)
FREQ = (ELF-ELI)/.4FNUZ
IF (FREQ.GT.FMAX.OR.FREQ.LT.FMIN) GO TO 7300
C
C****** LEVEL NAMES
C
KAF = KMAXF+2*(1-INOF)
KCF = J+1-KAF-MOD(ISYMF,2)
KAI = KMAXI+2*(1-INOI)
KCI = J+1-KAI-MOD(ISYMI,2)
C
C****** EIGEN VECTORS
C
CALL EIVEC(NHF,HD,HF,ELF,TVF)
CALL EIVEC(NHI,HDLO,HFLO,ELI,TVI)
C
C****** LINE STRENGTH
C
FAC = 0.0D0
NN = MINO(NHI,NHF)
DO 7520 II=1,NN
7520 FAC = FAC+CFACP(II)*TVF(II)*TVI(II)
IF (NTYPE.EQ.1) GO TO 7540
C
FACP = 0.0D0
IF (KMAXF.LT.J) GO TO 7510
NN = MINO(NHF-1,NHI)
IF (NN.LT.1) GO TO 7512
DO 7514 II=1,NN
7514 FACP = FACP+CFACP(II)*TVF(II+1)*TVI(II)
GOTO 7512
C
7510 NN = MINO(NHF,NHI-1)
IF (NN.LT.1) GO TO 7512
DO 7516 II=1,NN
7516 FACP = FACP+CFACP(II)*TVF(II)*TVI(II+1)
C
7512 IF (NTYPE.EQ.3) FACP = -FACP
FAC = FAC+FACP
C
7540 STRE = FAC**2*FLJIN
STRE=(STRE*DEXP((-ELI/(0.695*TT)))/ROTPF
KK=IABS(KAI-KCI)
IF(ISOTOPE.EQ.161) THEN
STNUC=(1.+2.*REAL(MOD(KK,2))))
ELSEIF(ISOTOPE.EQ.262) THEN
STNUC=(6.-3.*REAL(MOD(KK,2))))
ELSE
STNUC=1.0
ENDIF
STIMEM=(1.-DEXP(FCT*FREQ))
STRENGTH=STNUC*STRE
STRE=(STRENGTH*STIMEM*FREQ*BS)/(FNUZ*VIBPF)

C******STORE THE CALCULATED TRANSITION
C
  IF (STRE.GE.STMIN) CALL STORE(NLINE,J,KAF,KCF,J,KAI,
  1
    KCI,FREQ,STRENTYPE)

7300 CONTINUE
7200 CONTINUE
7100 CONTINUE
7000 CONTINUE

4200 CONTINUE

C

9000 CONTINUE

C****** SORT AND PRINTOUT THE CALCULATED SPECTRUM
C
PRINT OUT THE TOTAL NUMBER OF LINES MEETING THE STRENGTH
AND FREQUENCY RANGE CRITERIA.
C
WRITE(6,6013) NLINE
6013 FORMAT(10X,'TOTAL NUMBER OF LINES=',I6/)

ARRANGE THE STORED TRANSITIONS IN ORDER OF INCREASING
FREQUENCY.
C
CALL SORT(NLINE)
C
PRINT OUT THE TRANSITION TYPE AND QUANTUM STATE LABELS,
THE TRANSITION FREQUENCY, THE LINE STRENGTH AND
THE RELATIVE STRENGTH. DISABLE THIS SUBROUTINE CALL TO
SUPPRESS PRINTING.
C
CALL PRINT(NLINE)

PRINT OUT THE SUM OF STRENGTH WHICH INCLUDES ONLY THE
DIRECTION COSINE AND THE ROTATIONAL TERMS.
C
WRITE (6,6017) TOTINT
6017 FORMAT(10X,'TOTAL BAND INTENSITY=',1PE10.4/)
C
SORT THE STORED TRANSITIONS INTO FREQUENCY BINS OF WIDTH
EQUAL TO THE FREQUENCY RANGE DIVIDED BY NBINS.

32
CALL BINSORT(NLINE)

APPLY A GAUSSIAN LINE SHAPE OF HALFWIDTH = "WIDTH" TO THE SUMMED INTENSITY IN EACH BIN.

CALL SHAPE(NLINE)

STOP
END
PROGRAM ASYMEMS.FOR

IMPLICIT REAL*8(A-H,O-Z)

ASYMMETRIC ROTOR FREQUENCY ESTIMATION PROGRAM
FOR INFRARED AND VISIBLE SPECTROSCOPY
CODED BY Y.E.

MODIFIED BY C.H.D., R.T.L., H.H.N.

DIMENSION NAME(18), HD(50), HF(50), HDLO(50), HFLO(50),
1       EL(50), ELLO(50), CFAC(50), CFACP(50), TVF(50),
2       TVI(50), LTYPE(3), P(30)

LOGICAL LTYPE
COMMON /CON/ PAR(30)
COMMON /FREQ/ FMIN, FMAX
COMMON /BINS/ BIN(5000), BINEX(5000), NBINS, WIDTH
COMMON /OUTPUT/ ACCESS$, FILENAME$
COMMON /INTEN/ TOTINT, STRENGTH
CHARACTER*24 ACCESS$, FILENAME$
CHARACTER*8 ACCESS$, FILENAME$
INTEGER*2 IYEAR, IMONTH, IDAY, IHOUR, IMINUTE
CALL GETTIM(IHOUR, IMINUTE)
CALL GETDAT(IYEAR, IMONTH, IDAY)

ENTER NAME OF PARAMETER FILE TO BE USED AS INPUT

WRITE (6,*) 'ENTER INPUT FILE NAME?'
READ 99, FILENAME$
99 FORMAT (A8)

ENTER NAME OF FILE TO BE USED FOR STORAGE OF OUTPUT

WRITE (6,*) 'ENTER OUTPUT FILE NAME?'
READ 99, FILENAME$

THE INPUT PARAMETER FILE IS LOCATED ON DRIVE C: IN
SUBDIRECTORY ASYMRTR

THE OUTPUT FILE IS WRITTEN TO DRIVE A:

ACCESS$ = 'C:\ASYMRTR\FILENAME$\'.DAT'
ACCESS$ = 'A:\FILENAME$\'.DAT'
OPEN (2, FILE=ACCESS$, ACCESS='SEQUENTIAL')

ISOTOPE CODE IS READ:

161 = H2O
C 262 = D2O
C 162 = HDO
C
C READ(2,*) ISOTOPE
C
C THE VARIABLES ARE READ FROM THE PARAMETER FILE:
C
C \( \text{PAR}(1,2,3) = A, B, C \) VALUES FOR THE UPPER STATE
C \( \text{PAR}(4,5,6,7,8) = \text{CENTRIFUGAL DISTORTION CONSTANTS} \)
C FOR THE UPPER STATE
C \( \text{PAR}(10-15) = \text{UNUSED IN PRESENT VERSION; ALL = 0} \)
C \( \text{PAR}(16,17,18) = A, B, C \) VALUES FOR THE LOWER STATE
C \( \text{PAR}(19,20,21,22,23) = \text{CENTRIFUGAL DISTORTION} \)
C \( \text{CONSTANTS FOR THE LOWER STATE} \)
C \( \text{PAR}(24-30) = \text{UNUSED IN PRESENT VERSION; ALL = 0} \)
C
C DO 111 I=1,7,3
111 READ(2,*) (PAR(J), J=I,I+2)
C 67 FORMAT(3F16.8)
DO 121 I=10,15
121 PAR(I)=0.
DO 131 I=16,22,3
131 READ(2,*) (PAR(J), J=I,I+2)
DO 141 I=25,30
141 PAR(I)=0.
C
C READ NBINS = NUMBER OF BINS INTO WHICH FREQUENCY RANGE IS
C DIVIDED AND WIDTH = HALF-WIDTH OF GAUSSIAN LINE SHAPE
C
C READ (2,84) NBINS,WIDTH
84 FORMAT (I5,F10.6)
C
C READ IITY = BAND TYPE
C 100 = A TYPE BAND
C 010 = B TYPE BAND
C 001 = C TYPE BAND
C
C JMIN AND JMAX SET MINIMUM AND MAXIMUM VALUES OF J
C KTAU = MAXIMUM CHANGE ALLOWED IN TAU
C
C READ (2,69) IITY,JMIN,JMAX,KTAU
69 FORMAT (4I4)
C
C FMIN AND FMAX SET ALLOWED LIMITS FOR FREQUENCY RANGE
C IN CM\(^{-1}\). FNUZ IS THE BAND CENTER IN CM\(^{-1}\)
C
C READ (2,79) FMIN,FMAX,FNUZ
58 FORMAT(3F10.6)
C
C STMIN = MINIMUM STRENGTH FOR STORAGE OF LINE
C TT = TEMPERATURE
C BS = BAND STRENGTH FOR TRANSITION BEING CALCULATED
C
C READ(2,59) STMIN,TT,BS
59 FORMAT(E12.3,2F10.4)
FNU1, FNU2, FNU3 are the fundamental frequencies in CM-1

READ (2, 79) FNU1, FNU2, FNU3

FORMAT (3F10.4)
CLOSE (2)

The parameters read from the parameter file are printed out.

WRITE (6, 6019)
6019 FORMAT (10X, 'OUTPUT FROM PROGRAM ASMEMS.FOR'///)
WRITE (6, 6022) IMONTH, IDAY, IYEAR
6022 FORMAT (1X, I2, '/', I2, '/', I4)
WRITE (6, 6023) IHOUR, IMINUTE
6023 FORMAT (1X, I2, ':', I2/)  
WRITE (6, 6034) FILENAME
6034 FORMAT (' PARAMETER FILE ', A8//)
WRITE (6, 6036) FILENAME1$
6036 FORMAT (' OUTPUT FILE ', A8//)
WRITE (6, 6020) (PAR(I), I = 1, 8)
6020 FORMAT (' UPPER STATE CONSTANTS'//
1   ' A = ', F16.4, 5X, ' B = ', F16.4, 5X, ' C = ', F16.4/
2   ' DLJ = ', F16.8, 5X, ' DLJK = ', F16.8, 5X, ' DLK = ', F16.8/
3   ' DSJ = ', F16.8, 5X, ' DSK = ', F16.8//)
WRITE (6, 6025) (PAR(I), I = 16, 23)
6025 FORMAT (' LOWER STATE CONSTANTS'//
1   ' A = ', F16.4, 5X, ' B = ', F16.4, 5X, ' C = ', F16.4/
2   ' DLJ = ', F16.8, 5X, ' DLJK = ', F16.8, 5X, ' DLK = ', F16.8/
3   ' DSJ = ', F16.8, 5X, ' DSK = ', F16.8//)
DO 100 I = 1, 3
100 LTYPE(I) = .FALSE.
IF (ITY.GE.100) LTYPE(1) = .TRUE.
IF (MOD(ITY, 100).GE.10) LTYPE(2) = .TRUE.
IF (MOD(ITY, 10).GE.1) LTYPE(3) = .TRUE.
WRITE (6, 6030) LTYPE, JMIN, JMAX
6030 FORMAT (// ' SELECTION RULES ', 3L4/
1   ' J RANGE ', I4, ' TO ', I4)
WRITE (6, 6040) KTAU, FMIN, FMAX, FNUZ, FNU1, FNU2, FNU3,
1   STMIN, TT, NBINS, WIDTH, BS
6040 FORMAT (// ' MAX. DELTA TAU ', I4/
1   ' FREQ. RANGE ', F10.4, ' TO ', F10.4, ' CM-1'/
2   ' BAND ORIGIN ', F10.4, ' CM-1'/
7   ' NU #1 ', F10.4, ' CM-1'/
8   ' NU #2 ', F10.4, ' CM-1'/
9   ' NU #3 ', F10.4, ' CM-1'/
3   ' MIN. STRENGTH ', E12.3/
4   ' TEMPERATURE ', F7.2/
5   ' NBINS ', I5/
6   ' WIDTH ', F10.6/
7   ' BAND STRENGTH ', F10.4///)
SET LINE COUNTER TO ZERO
NLINE = 0
SET INITIAL TOTAL BAND INTENSITY = 0
TOTINT=0.0
DEFINE FCT = FACTOR FOR BOLTZMANN CALCULATIONS
FCT=-1.438786/TT
CALCULATE VIBRATIONAL PARTITION FUNCTION
VIBPF=1./(1.-DEXP(FCT*FNU1))*(1.-DEXP(FCT*FNU2))*(1.-DEXP(FCT*FNU3))
CALCULATE ROTATIONAL PARTITION FUNCTION
ROTPF=(TT**3/(PAR(16)*PAR(17)*PAR(18)))**.5
DO 9000 J=JMIN,JMAX
PRINT J ON SCREEN TO TRACK PROGRESS OF CALCULATION
PRINT 6010,J
6010 FORMAT (1X,I5)
C******  R BRANCH TRANSITIONS
IF (J.EQ.JMIN) GO TO 4000
FLJIN=1.DO/DBLE(J)
JLO = J-1
DO 2000 NTYPE=1,3
IF (.NOT.LTYPE(NTYPE)) GO TO 2000
DO 2100 ISYMF=1,4
ISYMI = ISEL(ISYMF,NTYPE,1)
CALL ECALC(0,ISYMF,J,HD,HF,EL,NHF,KMAXF,MAXT)
CALL ECALC(1,ISYMI,JLO,HDLO,HFLO,ELLO,NHI,KMAXI,MAXTLO)
IF (NHF*NHI.EQ.0) GO TO 2100
C******  CALCULATE DIRECTION COSINE
CALL CFACTR(1,NTYPE,NHF,NHI,KMAXF,KMAXI,J,CFAC,CFACP)
C***** RANGE OF ISHIFT
C
NTDEL = MAXT-MAXTLO
NSMAX = (KTAU-NTDEL+100)/4-25
NSMIN = 25-(KTAU+NTDEL+100)/4
C
DO 2200 ISHIFT=NSMIN,NSMAX
IF (ISHIFT.GE.0) GO TO 2180
N = MINO(NHF+ISHIFT,NHI)
IF (N.LT.1) GO TO 2200
NPLUSF = -ISHIFT
NPLUSI = 0
GO TO 2210
C
2180 N = MINO(NHF,NHI-ISHIFT)
IF (N.LT.1) GOTO 2200
NPLUSF = 0
NPLUSI = ISHIFT
2210 CONTINUE
C
C***** CALCULATE INDIVIDUAL TRANSITIONS
C
DO 2300 I=1,N
INOF = I+NPLUSF
INOI = I+NPLUSI
ELF = EL(INOF)
ELI = ELLO(INOI)
FREQ = (ELF-ELI)/1.+FNUZ
C
TEST WHETHER LINE POSITION IS WITHIN SPECIFIED FREQUENCY
C RANGE. IF SO, CONTINUE WITH INTENSITY CALCULATION;
C IF NOT, CALCULATE NEXT LINE.
C
IF (FREQ.GT.FMAX.OR.FREQ.LT.FMIN) GO TO 2300
C
C***** LEVEL NAMES
C
KAF = KMAXF+2*(1-INOF)
KCF = J+1-KAF-ISYMF+2*(ISYMF/2)
KAI = KMAXI+2*(1-INOI)
KCI = JLO+1-KAI-ISYMIf2*(ISYMIf2)
C
C***** CALCULATE EIGEN VECTORS
C
CALL EIVEC(NHF,HD,HF,ELF,TVF)
CALL EIVEC(NHI,HDLO,HFLO,ELI,TVI)
C
C***** CALCULATE LINE STRENGTH
C
FAC = 0.0D0
IPLUS = 0
IF (KMAXF-KMAXI.EQ.2) IPLUS = 1
NN = MIN0(NHF-IPLUS,NHI)
DO 2520 II=1,NN
2520 FAC = FAC+CFAC(II)*TVF(II+IPLUS)*TVI(II)
IF (NTYPE.EQ.1) GOTO 2540
FACP = 0.0DO
NN = MIN0(NHF-1,NHI)
IF (NN.LT.1) GO TO 2512
DO 2530 II=1,NN
2530 FACP = FACP+CFACP(II)*TVF(II+1)*TVI(II)
2512 IF (NTYPE.EQ.2) FACP = -FACP
FAC = FAC+FACP
2540 STRE = FAC**2*FLJIN
C
C MULTIPLY DIRECTION COSINES FACTOR BY ROTATIONAL BOLTZMANN
C FACTOR OVER ROTATIONAL PARTITION FUNCTION
C
STRE=(STRE*DEXP(-ELF/(0.695*TT)))/ROTPF
C
ASSIGN NUCLEAR STATISTICS FACTOR BASED ON IDENTITY OF
C ISOTOPE AND WHETHER LEVEL IS ODD OR EVEN
C
H2O   1:3 FOR EVEN:ODD
D2O   6:3 FOR EVEN:ODD
HDO   1 FOR ALL LEVELS
C
KK=IABS(KAF-KCF)
IF(ISOTOPE.EQ.161) THEN
STNUC=(1.+2.*(REAL(MOD(KK,2)))
ELSEIF(ISOTOPE.EQ.262) THEN
STNUC=(6.-3.*(REAL(MOD(KK,2)))
ELSE
STNUC=1.0
ENDIF
C
STIMULATED EMISSION IS NOT USED IN EMISSION CALCULATION
C
STIMEM=(1.-DEXP(FCT*FREQ))
C
CALCULATE STRENGTH WHICH INCLUDES ROTATIONAL AND NUCLEAR
C STATISTICS FACTORS. THIS WILL BE USED LATER TO NORMALIZE
C FOR COMPARISON OF DIFFERENT ISOTOPES. TOTINT IS SUM OF
C STRENGTH FOR EACH LINE.
C
STRENGTH=STNUC*STRE
C
CALCULATE FINAL INTENSITY BY MULTIPLYING BY FREQUENCY**4,
C BAND STRENGTH, VIBRATIONAL BOLTZMANN FACTOR, AND DIVIDING
C BY VIBRATIONAL PARTITION FUNCTION AND BAND CENTER.
C
STRE=(STRENGTH*(FREQ**4)*BS*DEXP(-(FNUZ)/(0.695*TT)))/
1 (VIBPF*FNUZ)
C
C***** STORE THE CALCULATED TRANSITION IF STRE EXCEEDS THE
C MINIMUM STRENGTH CRITERION.
IF (STRE.GE.STMIN) CALL STORE(NLINE,J,KAF,KCF,JLO,KAI,
   KCI,FREQ,STRE,NTYPE)
2300 CONTINUE
2200 CONTINUE
2100 CONTINUE
2000 CONTINUE

C***** P BRANCH TRANSITIONS - P BRANCH TRANSITION FREQUENCIES

AND STRENGTHS ARE CALCULATED BY THE SAME METHOD USED

ABOVE FOR THE R BRANCH TRANSITIONS.

4000 CONTINUE

IF (J.EQ.JMIN) GO TO 4200
FLJIN = 1.DO/DBLE(J)
JLO = J-1

DO 3000 NTYPE=1,3
IF (.NOT.LTYPE(NTYPE)) GO TO 3000

DO 3100 ISYMF=1,4
ISYMI = ISEL(ISYMF,NTYPE,1)
CALL ECALC(1, ISYMF,J,HD,HF,EL,NHF,KMAXF,MAXT)
CALL ECALC(0,ISYMI,JLO,HDLO,HFLO,ELLO,NHI,KMAXI,MAXTLO)
IF (RHF*NHI.EQ.0) GO TO 3100

C***** CALCULATE DIRECTION COSINES

CALL CFACTR(1,NTYPE,NHF,NHI,KMAXF,NMAXI,CFAC,CFACP)

C***** RANGE OF ISHIFT

NTDEL = MAXT-MAXTLO
NSMAX = (KTAU-NTDEL+100)/4-25
NSMIN = 25-(KTAU+NTDEL+100)/4

DO 3200 ISHIFT=NSMIN,NSMAX
IF (ISHIFT.GE.0) GO TO 3180
N = MINO(NHF+ISHIFT,NHI)
IF (N.LT.1) GOTO 3200
NPLUSF = -ISHIFT
NPLUSI = 0
GOTO 3210

3180 N = MINO(NHF,NHI-ISHIFT)
IF (N.LT.1) GOTO 3200
NPLUSF = 0
NPLUSI = ISHIFT

40
CONTINUE
C
***** CALCULATE INDIVIDUAL TRANSITIONS
C
DO 3300 I=1,N
INOF = I+NPLUSF
INOI = I+NPLUSI
ELF = EL(INOF)
ELI = ELLO(INOI)
FREQ = (ELI-ELF)/1.+FNUZ
IF (FREQ.GT.FMAX.OR.FREQ.LT.FMIN) GO TO 3300
C
***** LEVEL NAMES
C
KAF = KMAXF+2*(1-INOF)
KCF = J+1-KAF-ISYM+2*(ISYM/2)
KAI = KMAXI+2*(1-INOI)
KCI = JLO+1-KAI-ISYMI+2*(ISYMI/2)
C
***** CALCULATE EIGEN VECTORS
C
CALL EIVEC(NHF,HD,HF,ELF,TVF)
CALL EIVEC(NHI,HDLO,HFLO,ELI,TVI)
C
***** CALCULATE LINE STRENGTH
C
FAC = 0.0D0
IPLUS = 0
IF (KMAXF-KMAXI.EQ.2) IPLUS = 1
NN = MIN0(NHF-IPLUS,NHI)
DO 3520 II=1,NN
3520 FAC = FAC+CFAC(II)*TVF(II+IPLUS)*TVI(II)
IF (NTYPE.EQ.1) GOTO 3540
FACP = 0.0D0
NN = MIN0(NHF-1,NHI)
IF (NN.LT.1) GO TO 3512
DO 3530 II=1,NN
3530 FACP = FACP+CFACP(II)*TVF(II+1)*TVI(II)
3512 IF (NTYPE.EQ.2) FACP = -FACP
FAC = FAC+FACP
3540 STRE = FAC**2*FLJIN
STRE=(STRE*DEXP(-ELF/(0.695*TT)))/ROTPF
KK=IABS(KAF-KCF)
IF(ISOTOPE.EQ.161) THEN
STNUC=(1.+2.*(REAL(MOD(KK,2))))
ELSEIF(ISOTOPE.EQ.262) THEN
STNUC=(6.-3.*(REAL(MOD(KK,2))))
ELSE
STNUC=1.0
ENDIF
C
STIMEM=(1.-DEXP(FCT*FREQ))
STRENGTH=STNUC*STRE
STRE=(STRENGTH*(FREQ**4)*BS*DEXP(-(FNUZ)/(0.695*TT))))/41
(VIBPF*FNUZ)

C***** STORE THE CALCULATED TRANSITION
C
IF (STRE.GE.STMIN) CALL STORE(NLINE,JLO,KAI,KCI,J,KAF,
1 KCF,FREQ,STRE,NTYPE)
C
3300 CONTINUE
3200 CONTINUE
3100 CONTINUE
3000 CONTINUE
C
4100 CONTINUE
C
C***** Q BRANCH TRANSITIONS -.Q BRANCH TRANSITION FREQUENCIES
C AND LINE STRENGTHS ARE CALCULATED BY THE SAME METHOD
C USED ABOVE FOR THE P AND R BRANCHES.
C
IF (J.EQ.0) GOTO 4200
FLJIN = DBLE(J+J+1)/DBLE(J*(J+1))
C
DO 7000 NTYPE=1,3
IF (.NOT.LTYPE(NTYPE)) GO TO 7000
C
DO 7100 'ISYMF=1,4
ISYMI = ISEL(ISYMF,NTYPE,0)
CALL ECALC(0,ISYMF,J,HD,HF,EL,NHF,KMAXF,MAXT)
CALL ECALC(1,ISYMI,J,HDLO,HFLO,ELLO,NHI,KMAXI,MAXTLO)
IF (NHF*NHI.EQ.0) GO TO 7100
C
C*****CALCULATE DIRECTION COSINES
C
CALL CFACTR(0,NTYPE,NHF,NHI,KMAXF,KMAXI,J,CFAC,CFACP)
C
C***** RANGE OF ISHIFT
C
NTDEL = MAXT-MAXTLO
NSMAX = (KTAU-NTDEL+100)/4-25
NSMIN = 25-(KTAU+NTDEL+100)/4
C
DO 7200 ISHIFT=NSMIN,NSMAX
C
IF (ISHIFT.GE.0) GO TO 7320
N = MIN0(NHF+ISHIFT,NHI)
IF (N.LT.1) GO TO 7200
NPLUSF = -ISHIFT
NPLUSI = 0
GO TO 7330

42
C 7320 N = MIN0(NHF,NHI-ISHIFT)
   IF (N.LT.1) GO TO 7200
   NPLUSF = 0
   NPLUSI = ISHIFT
C
C***** INDIVIDUAL TRANSITIONS
C
7330 DO 7300 I=1,N
   INOF = I+NPLUSF
   INOI = I+NPLUSI
   ELF = EL(INOF)
   ELI = ELLO(INOI)
   FREQ = (ELF-ELI)/1.+FNUZ
   IF (FREQ.GT.FMAX.OR.FREQ.LT.FMIN) GO TO 7300
C
C***** LEVEL NAMES
C
   KAF = KMAXF+2*(1-INOF)
   KCF = J+1-KAF-MOD(ISYMf,2)
   KAI = KMAXI+2*(1-INOI)
   KCI = J+1-KAI-MOD(ISYMl,2)
C
C*****EIGEN VECTORS
C
   CALL EIVEC(NHF,HD,HF,ELF,TVF)
   CALL EIVEC(NHI,HDLO,HFL,ELI,TVI)
C
C*****LINE STRENGTH
C
   FAC = 0.0D0
   NN = MIN0(NHI,NHF)
   DO 7520 II=1,NN
    7520 FAC = FAC+CFAC(II)*TVF(II)*TVI(II)
   IF (NTYPE.EQ.1) GO TO 7540
C
   FACP = 0.0D0
   IF (KMAXF.LT.J) GO TO 7510
   NN = MIN0(NHF-1,NHI)
   IF (NN.LT.1) GO TO 7512
   DO 7514 II=1,NN
   7514 FACP = FACP+CFACP(II)*TVF(II+1)*TVI(II)
   GOTO 7512
C
   7510 NN = MIN0(NHF,NHI-1)
   IF (NN.LT.1) GO TO 7512
   DO 7516 II=1,NN
   7516 FACP = FACP+CFACP(II)*TVF(II)*TVI(II+1)
C
   7512 IF (NTYPE.EQ.3) FACP = -FACP
   FAC = FAC+FACP
C
   7540 STRE = FAC**2*FLJIN
STRE = (STRE * DEXP(-ELF/(0.695*TT))) / ROTPF
KK = IABS(KAF - KCF)
IF (ISOTOPE.EQ.161) THEN
  STNUC = (1. + 2. * (REAL(MOD(KK,2))))
ELSEIF (ISOTOPE.EQ.262) THEN
  STNUC = (6. - 3. * (REAL(MOD(KK,2))))
ELSE
  STNUC = 1.0
ENDIF
C
STIMEM = (1. - DEXP(FCT*FREQ))
STRENGTH = STNUC * STRE
STRE = (STRENGTH * (FREQ**4) * BS * DEXP(-(FNUZ)/(0.695*TT))) / (VIBPF * FNUZ)
C
**** STORE THE CALCULATED TRANSITION
C
IF (STRE .GE. STMIN) CALL STORE(NLINE, J, KAF, KCF, J, KAI, 1, KCI, FREQ, STRE, NTYPE)
C
7300 CONTINUE
7200 CONTINUE
7100 CONTINUE
7000 CONTINUE
C
4200 CONTINUE
C
9000 CONTINUE
C
C
**** SORT AND PRINTOUT THE CALCULATED SPECTRUM
C
PRINT OUT THE TOTAL NUMBER OF LINES MEETING THE STRENGTH AND FREQUENCY RANGE CRITERIA.
WRITE(6,6013) NLINE
6013 FORMAT(10X,'TOTAL NUMBER OF LINES = ',I6)
C
ARRANGE THE STORED TRANSITIONS IN ORDER OF INCREASING FREQUENCY.
CALL SORT(NLINE)
C
CALL PRINT(NLINE)
C
PRINT OUT THE SUM OF STRENGTH WHICH INCLUDES ONLY THE DIRECTION COSINE AND THE ROTATIONAL TERMS.
WRITE (6, 6017) TOTINT
6017 FORMAT(10X, 'TOTAL BAND INTENSITY = ', 1PE10.4/)

C
C SORT THE STORED TRANSITIONS INTO FREQUENCY BINS OF WIDTH
C EQUAL TO THE FREQUENCY RANGE DIVIDED BY NBINS.
C
CALL BINSORT(NLINE)

C
C APPLY A GAUSSIAN LINE SHAPE OF HALFWIDTH = "WIDTH" TO THE
C SUMMED INTENSITY IN EACH BIN.
C
CALL SHAPE(NLINE)

C
STOP
END
C  ASYMSUB.FOR

INTEGER FUNCTION ISEL(ISYM,NTYPE,IQR)

DIMENSION ITBL(4,3,2)
DATA ITBL/ 2,1,4,3, 3,4,1,2, 4,3,2,1,
1 1,2,3,4, 4,3,2,1, 3,4,1,2/
ISEL = ITBL(ISYM,NTYPE,IQR+1)
RETURN
END

SUBROUTINE CFACTR(IQR,NTYPE,NHF,NHI,KMAXF,KMAXI,J,
1CFAC,CFACP)
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION CFAC(50),CFACP(50)

C THIS ROUTINE CALCULATES THE DIRECTION COSINES
C J NUMBER OF I STATE SHOULD BE LESS THAN OR EQUAL TO
C THAT OF F STATE
C
N = MIN0(NHF,NHI)

IF (IQR.EQ.0) GO TO 1000

C***** P,R BRANCH
KP = KMAXI+2
IF (NTYPE.NE.1) GO TO 910

C***** A TYPE TRANSITION
JJ = J*J
DO 920 I=1,N
K = KP-2*I
920 CFAC(I) = DSQRT(DBLE(JJ-K*K))
RETURN

C***** B,C TYPE TRANSITIONS

910 DO 940 I=1,N
K = KP-2*I
W = (J+K)*(J+K+1)
IF (K.EQ.0) W = W+W
940 CFAC(I) = 0.5D0*DSQRT(W)

N = MIN0(NHF-1,NHI)
IF (N.LE.0) RETURN
KP = KP-1
DO 950 I=1,N
K = KP-2*I
W = (J-K)*(J-K-1)
IF (K.EQ.0) W = W+W
950 RETURN
950     CFACP(I) = 0.5D0*DSQRT(W)
     RETURN

C****** Q BRANCH
C
1000     KP = KMAXF+2
     IF (NTYPE.NE.1) GO TO 1160
C
C****** A TYPE TRANSITION
C
     DO 1170 I=1,N
1170     CFAC(I) = KP-2*I
     RETURN
C
C****** B,C TYPE TRANSITIONS
C
1160     JJ = J*(J+1)
     IF (KMAXF.LT.J) GO TO 1190
     KP = KP-1
     NP = MINO(NHF-1,NHI)
     GO TO 1165
1190     NP = MINO(NHF,NHI-1)
C
1165     DO 1120 I=1,N
     K = KP-2*I
     W = JJ-K*(K+1)
     IF (K.EQ.0) W = W+W
1120     CFAC(I) = 0.5D0*DSQRT(W)
C
     IF (NP.LT.1) RETURN
     KP = KP-1
     DO 1125 I=1,NP
     K = KP-2*I
     W = JJ-K*(K+1)
     IF (K.EQ.0) W = W+W
1125     CFACP(I) = 0.5D0*DSQRT(W)
     RETURN
END

SUBROUTINE ECALC(IUL, ISYM,J,HD,HF,EL,NH,KMX,MT)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON /CON/
     PAR(30)
/CONST/ P(15)
DIMENSION HD(50),HF(50),EL(50),HF1(50)
C
     IF (J.LE.98) GO TO 100
     NH = 0
     RETURN
C
100     DO 110 I=1,15
110     P(I) = PAR(I+15*IUL)
C
     CALL MATRIX(ISYM,HD,HF,NH,KMX,J)
     IF (NH.EQ.0) RETURN
EL(NH) = HD(NH)
DO 200 I=1,NH-1
HF1(I) = HF(I)**2
EL(I) = HD(I)
CONTINUE

IF (NH.NE.1) CALL DTSM(NH,EL,HF1)
MT = 3*J-ISYM+1-(J/2)*4
IF (MT.GT.J) MT = MT-4
RETURN
END

SUBROUTINE STORE(NLINEJKAF,KCFJLKAIKCI,FREQ,ISTRE,NTYPE)
IMPLICIT REAL*8(A-H,O-Z)
C
THIS ROUTINE STORES THE FREQUENCY, STRENGTH, AND LEVEL NAME OF ALL TRANSITIONS MEETING THE STRENGTH AND FREQUENCY RANGE CRITERIA.
COMMON /TBL/ NLEV(10000),FRQ(10000),ST(10000)
COMMON/TOTINT,STRENGTH
C
THE LINE COUNTER NLINE IS ADVANCED AS EACH ADDITIONAL LINE IS STORED.
NLINE = NLINE+1
NO MORE THAN 10,000 LINES MAY BE STORED
IF (NLINE.GT.10000) RETURN
FRQ(NLINE) = FREQ
ST(NLINE) = STRE
NLEV(NLINE) = ((J*100+KAF)*2+(KCF+KAF-J))*100000
1 +((JL*100+KAI)*2+(KCI+KAI-JL))*5
2 +NTYPE
C
STRENGTH IS SUMMED TO GIVE TOTINT.
TOTINT=TOTINT+STRENGTH
RETURN
END

SUBROUTINE SORT(NLINE)
C
C
THIS ROUTINE SORTS THE STORED TRANSITIONS BY FREQUENCY AND STORES THEM AGAIN IN ORDER OF INCREASING WAVENUMBER.
IMPLICIT REAL*8(A-H,O-Z)
COMMON /TBL/ NLEV(10000),FRQ(10000),ST(10000)
COMMON/TOTINT,STRENGTH
C
LOGNB2 = INT((ALOG(FLOAT(NLINE))/ALOG(2.0))+1.E-5)
M=NLINE

48
DO 49 NN = 1,LOGNB2
M=M/2
K = NLINE - M
DO 44 J = 1,K
I = J
3 CONTINUE
L = I+M
IF (FRQ(L).LT.FRQ(I)) THEN
  F =FRQ(I)
  S =ST(I)
  N =NLEV(I)
FRQ(I)=FRQ(L)
FRQ(L)=F
ST(I)=ST(L)
ST(L)=S
NLEV(I)=NLEV(L)
NLEV(L)=N
I = I-M
IF (I.GE.1) GOTO 3
ENDIF
44 CONTINUE
49 CONTINUE
C
C THIS LOOP NORMALIZES EACH ISOTOPE SO THAT THE SUM OF
C TOTINT IS EQUAL TO 1. THIS IS DONE BY DIVIDING THE
C STRENGTH OF EACH LINE BY TOTINT.
C
DO 8005 I=1,NLINE
ST(I)=ST(I)/TOTINT
8005 CONTINUE
RETURN
END
SUBROUTINE PRINT(NLINE)

C THIS ROUTINE PRINTS THE TRANSITION LABELS, FREQUENCY,
C STRENGTH, AND RELATIVE STRENGTH FOR EACH LINE.
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON /TBL/ NLEV(10000),FRQ(10000),ST(10000)
DIMENSION INTYPE(3),ITYP(3)
* DATA INTYPE/IHA,IHB,IHC/, ITYP/IHP,IHQ,IHR/
C
C SMAX, USED TO CALCULATE RELATIVE STRENGTH, IS
C INITIALIZED TO 0.
C
SMAX = 0.0DO
DO 100 I=1,NLINE
IF (SMAX.LT.ST(I)) SMAX=ST(I)
100 CONTINUE
C
C DO 200 I=1,NLINE

49
N = NLEV(I)
NTYPE = MOD(N, 5)
N = N/5
M = MOD(N, 20000)
N = N/20000
J = N/200
KAF = MOD(N/2, 100)
KCF = J-KAF+MOD(N, 2)
JLO = M/200
KAI = MOD(M/2, 100)
KCI = JLO-KAI+MOD(M, 2)
RST = ST(I)/SMAX

C
IQR = 1
IF (J.EQ.JLO) IQR=2
IF (J.GT.JLO) IQR=3

C
WRITE(6, 1000) INTYPE(NTYPE), ITYP(IQR), J, KAF, KCF, JLO,
KAI, KCI, FRQ(I), ST(I), RST
200 CONTINUE
RETURN
C
1000 FORMAT(5X, A1, 3X, A1, 3X, 3I3, 5X, 3I3, F16.5, 3X, 1PE10.3, 0PF8.4)
END

SUBROUTINE EIVEC(NS, A, B, ENERGY, T)
C CALCULATION OF EIGENVECTOR
IMPLICIT REAL*8 (A-H, O-Z)
C A DIAGONAL ELEMENTS OF TRIDIAGONAL MATRIX (LARGEST TO SMALLER)
C B OFF DIAGONAL ELEMENTS
DIMENSION A(50), B(50), T(50)
IF (NS.GT.1) GO TO 100
T(1) = 1.0D0
RETURN
100 WORK = DABS(A(1)-ENERGY)
NU = 1
DO 10 I=2, NS
WORKP = DABS(A(I)-ENERGY)
IF (WORKP.GT.WORK) GO TO 10
WORK = WORKP
NU = I
10 CONTINUE
C CALCULATE RATIO OF EIGENVECTOR
IF (NU.GT.1) T(1) = -B(1)/(A(1)-ENERGY)
IF (NU.LE.2) GO TO 18
DO 17 J=2, NU-1
17 T(J) = -B(J)/(B(J-1)*T(J-1)+A(J)-ENERGY)
18 IF (NU.LT.NS) T(NS) = -B(NS-1)/(A(NS)-ENERGY)
IF (NU.GE.NS-1) GO TO 20
K = NS-1-NU
DO 19 J=1, K
JA = NS-J
CONTINUE
19 \( T(JA) = -B(JA-1)/(B(JA) \times T(JA+1) - A(JA) - \text{ENERGY}) \)

C CALCULATE EIGEN-VECTOR

20 \( T(NU) = 1.0 \)

21 \( T2 = T(NU)^2 \)

22 IF(NU.EQ.1) GO TO 22

DO 21 J=1,NU-1

JA=NU-J

T(JA)=T(JA+1)*T(JA)

T2=T2+T(JA)**2

DO 24 J=NU+1,NS

T(J)=T(J-1)*T(J)

T2=T2+T(J)**2

T2=1.0/DSQRT(T2)

DO 25 J=1,NS

T(J)=T(J)*T2

RETURN

END

SUBROUTINE DTSM(NS,Q,E)

C DIAGONALIZATION OF TRIDIAGONAL MATRIX

IMPLICIT REAL*8(A-H,O-Z)

C Q  DIAGONAL FROM THE LARGEST ELEMENT TO SMALLER

C NS MUST BE LARGER THAN 1

DIMENSION Q(50),E(50)

C E  (OFFSET-DIAGONAL ELEMENT)**2

PASS=0.1D-4

E(NS)=0.0

C=0.0

NR=NS

C SHIFT ORIGIN

5 RE2=DSQRT(E(1))

CM=Q(1)-RE2

DO 6 I=2,NR

RE1=RE2

RE2=DSQRT(E(I))

CMP=Q(I)-RE1-RE2

IF(CM.GT.CMP)CM=CMP

CONTINUE

DO 7 I=1,NS

7 Q(I)=Q(I)-CM

C=C+CM

DO 8 I=2,NR

E(I-1)=E(I-1)/Q(I-1)

8 Q(I)=Q(I)-E(I-1)

C REPEAT ORTHOGONAL TRANSITION

NROT=0

11 IF(NROT.GE.10) GO TO 102

NROT=NROT+1

9 Q(I)=Q(I)+E(I)

DO 9 I=2,NR

E(I-1)=Q(I)*E(I-1)/Q(I-1)

9 Q(I)=Q(I)-E(I-1)+E(I)

IF(E(NR-1)-PASS) 103,11,11
DO 12 I=1,NR-1
Q(I)=Q(I)+E(I)
12 E(I)=E(I)*Q(I+1)
GO TO 5

NR=NR-1
E(NR)=0.0
IF(NR.GT.1) GO TO 102

DO 10 I=1,NS
Q(I)=Q(I)+C
RETURN

END

CONSTRUCTION OF TRIDIAGONAL MATRIX
SUBROUTINE MATRIX(ISYM,HDISYM,HOISYM,NH,KMAX,J)
IMPLICIT REAL*8(A-H,O-Z)
COMMON/CONST/A,B,C,DLJ,DLJK,DLK,DSJ,DSK,HLJ,HLJK,HLKJ,
1 HLK,HSJ,HSJK,HSK
DIMENSION HDISYM(50),HOISYM(50)
KPAR=(ISYM-1)/2
KMAX=(J+KPAR)/2-2-KPAR
NH=(KMAX+2)/2
IF(ISYM.EQ.2) NH=NH-1
IF(NH.LE.0) NH=0
IF(NH.EQ.0) RETURN

JP=J*(J+1)
BAVE = 0.500*(B+C)
AP=A-BAVE
BDIF =0.2500*(B-C)
FIJP =JP
ADD=((HSJ*FLJP-DSJ+HSJK)*FLJP+BDIF-DSK+HSK)*FLJP
BJJ=((HLJ*FLJP-DLJ)*FLJP+BAVE)*FIJP
BJJ2=(HLJK*FLJP-DLJK)*FIJP+AP
BJJ4=HLKJ*FLJP-DLK
DO 10 I=1,NH
K=KMAX+2-2*I
FLKX=K*K
HD=((HLK*FLKK+BJJ4)*FLKK+BJJ2)*FLKK+BJJ
IF(K.NE.1) GO TO 10
IF(ISYM.EQ.3) HD=HD+ADD
IF(ISYM.EQ.4) HD=HD-ADD
10 HDISYM(I)=HD
RETURN

END
SUBROUTINE SHAPE(NLINE)

THIS ROUTINE APPLIES A GAUSSIAN WITH HALFWIDTH = "WIDTH" TO EACH BIN. AFTER THE LINESHAPE APPLICATION, IT WRITES THE OUTPUT FILE CONTAINING THE LIMITS OF THE FREQUENCY RANGE, NBINS, AND THE INTENSITY FOR EACH BIN.

REAL INTEN,NORM
IMPLICIT REAL*8(A-H,O-Z)
COMMON /TBL/ NL Foo(l0000),FRQ(l0000),ST(l0000)
COMMON /FREQ/ FM IN,MAX
COMMON /BINS/ BINS(5000),BINDEX(5000),NBINS,W IDTH
COMMON/OTP/ACCESS2S
COMMON/INTEN,TOTINT
DIMENSION IN TEN(200),SM O O(5000)
CHARACTER*24 ACCESS2S
OPEN (8,FILE=ACCESS2S,STATUS='NEW',ACCESS=
1)'SEQUENTIAL')
WRITE (8,2006) ID INT(FMIN),ID INT(FMAX)
WRITE (6,2006) ID INT(FMIN),ID INT(FMAX)
WRITE(8,2007) NBINS

2007 FORMAT(I5)
2006 FORMAT(I5,1H,,I5)
NORM=SQR T(2.*AL OG(2.))/(WIDTH+1E-06)
STEP= (FMAX-FMIN)/FLOAT(NBINS) * NORM
X=STEP/2.

2009 FORMAT(1PE10.4)
INTEN(1)=GAUSS(X)*2.
SUM=INT EN(1)
G=INTEN(1)/2.
M=MIN1(200,((5.0/SNGL(STEP))+1.))
DO 20 J=2,M
X=X+STEP
INTEN(J)=G
G=GAUSS(X)
INTEN(J)=G+INTEN(J)
20 SUM=SUM+2.*INTEN(J)
BIG=0.0
DO 50 I=1,NBINS
SMO OTH(I)=BINST(I)*INTEN(1)
DO 40 J=2,M
K=I+J-1
IF(K.LE.NBINS)SMOOTH(I)=SMOOTH(I)+BINST(K)*INTEN(J)
K=I-J+1
40 IF(K.GE.1) SMOO OTH(I)=SMOOTH(I)+BINSTM(K)*INTEN(J)
2002 FORMAT(I4,5X,F10.4,5X,F10.4)
2005 FORMAT(1PE9.3)
50 CONTINUE

C TOTSMO IS THE SUM OF THE INTENSITIES IN ALL BINS AFTER THE GAUSSIAN LINESHAPE HAS BEEN APPLIED. BIG IS THE MAXIMUM INTENSITY IN ANY OF THE BINS.
TOTSMO=0.0
DO 49 I=1,NBINS
   TOTSMO=TOTSMO+SMOOTH(I)
   IF(SMOOTH(I).GE.BIG) BIG=SMOOTH(I)
C
   THE INTENSITY IN EACH BIN SMOOTH(I) IS WRITTEN TO THE
   OUTPUT FILE.

   WRITE(8,2005) SMOOTH(I)
   WRITE(6,2011) TOTSMO
   WRITE(6,2012) BIG
   2012 FORMAT(10X,'MAXIMUM INTENSITY = ',1PE10.4/)
   2011 FORMAT(10X,'TOTAL BAND INTENSITY(GAUSSIAN SUM) = ',
         11PE10.4/)
   CLOSE(8)
RETURN
END

REAL FUNCTION GAUSS(X)
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION B(5)
DATA B/1.3302744,-1.821256,1.7814779,-.35656378,.3193815/,
     DATA P/.2316419/,Q/.39894228/
T=1./(1.+P*X)
PROD=0.0
DO 10 I=1,5
   PROD=T*(B(I)+PROD)
   10 FORMAT(3F10.6)
GAUSS=0.5-Q*PROD*EXP(-(X**2/2.0))
RETURN
END
SUBROUTINE BINSORT(NLINE)

THIS ROUTINE SORTS THE STORED TRANSITIONS INTO BINS OF EQUAL WIDTH AND SUMS THE INTENSITY IN EACH BIN.

IMPLICIT REAL*8(A-H,O-Z)
COMMON /TBL/ NLEV(10000),FRQ(10000),ST(10000)
COMMON /FREQ/ FMIN,FMAX
COMMON /BINS/ BINST(5000),BINDEX(5000),NBINS,WIDTH

THE BIN WIDTH DEL IS CALCULATED BY DIVIDING THE FREQUENCY RANGE INTO NBINS EQUAL INCREMENTS.

DEL=(FMAX-FMIN)/FLOAT(NBINS)
K=1
DO 100 I=1,NBINS
  BINST(I)=0.
  BINDEX(I)= FMIN+REAL(I*DEL)
DO 200 J=K,NLINE
  IF(FRQ(J).LE.BINDEX(I)) THEN
    BINST(I) = BINST(I) + ST(J)
  ENDIF
  IF(FRQ(J).GT.BINDEX(I)) K=J
150 CONTINUE
100 CONTINUE
IF(FRQ(J).GT.BINDEX(I)) K=J
200 CONTINUE
150 CONTINUE
100 CONTINUE
110 DO 50 L=I+1,NBINS
  BINST(L)=0.
50 CONTINUE
RETURN
END
SAMPLE PARAMETER FILE FOR CO2

FNU1[F16.8]  FNU2[F16.8]  FNU3[F16.8]
FNUZ[F16.8]  FLOW[F16.8]  FHIGH[F16.8]
SV[F16.8]  TT[F16.8]
NBINS[I5]  WIDTH[F10.6]

ID = identification code
BU,DU,HU = upper state constants
BUQ,DUQ,HUQ = upper state constants for other doublet level
BL_DL,HL = lower state constants
JMIN,JMAX = minimum and maximum values of J
FMIN,FMAX = minimum and maximum values of frequency
FNU1,FNU2,FNU3 = fundamental frequencies
FNUZ = band center
FLOW = lower state vibrational frequency
FHIGH = upper state vibrational frequency
SV = band strength
TT = temperature
NBINS = number of bins
WIDTH = Gaussian halfwidth
<table>
<thead>
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<th>SAMPLE INPUT FILE CO2NU3</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
</tr>
<tr>
<td>0.38714069</td>
</tr>
<tr>
<td>1.32873E-7</td>
</tr>
<tr>
<td>0.077E-13</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
</tr>
<tr>
<td>0.39021817</td>
</tr>
<tr>
<td>1.33204E-7</td>
</tr>
<tr>
<td>0.055E-13</td>
</tr>
<tr>
<td>0 20 2000.</td>
</tr>
<tr>
<td>2500.</td>
</tr>
<tr>
<td>1388.1847</td>
</tr>
<tr>
<td>667.3801</td>
</tr>
<tr>
<td>2349.1433</td>
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<tr>
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<tr>
<td>955900.</td>
</tr>
<tr>
<td>296.</td>
</tr>
<tr>
<td>5000 2.0</td>
</tr>
</tbody>
</table>
OUTPUT FROM PROGRAM CO2ABS

5/28/1987
13: 6

INPUT FILE = CO2NU3
OUTPUT FILE = CO2ANU3

ID = 11

UPPER STATE CONSTANTS
B = 0.38714069 D = 1.3287E-07 H = 7.7000E-15

UPPER STATE CONSTANTS(OTHER DOUBLET LEVEL)
B = 0.00000000 D = 0.00000E-01 H = 0.00000E-01

LOWER STATE CONSTANTS
B = 0.39021817 D = 1.3320E-07 H = 5.5000E-15

J RANGE 0 TO 20
FREQUENCY RANGE 2000.0000 TO 2500.0000

BAND ORIGIN 2349.1433 CM-1
NU1 1388.1847 CM-1
NU2 667.3801 CM-1
NU3 2349.1433 CM-1

LOWER STATE VIBRATIONAL ENERGY = 0.0000 CM-1
UPPER VIBRATIONAL STATE ENERGY = 2349.1433 CM-1

BAND STRENGTH 955900.00000000
TEMPERATURE 296.0000
NBINS 5000
WIDTH 2.000000

P 20 2332.3694 1.128E+04 8.776261
P 18 2334.1569 1.178E+04 9.164751
P 16 2335.9199 1.197E+04 9.309935
P 14 2337.6586 1.179E+04 9.169426
P 12 2339.3728 1.120E+04 8.713461
P 10 2341.0625 1.019E+04 7.928887
P  8 2342.7277 8.770E+03 6.821999
P  6 2344.3685 6.968E+03 5.419867
P  4 2345.9847 4.846E+03 3.769805
P  2 2347.5763 2.490E+03 1.936939
R  0 2349.1716 1.261E+03 0.980531
R  2 2351.4477 3.741E+03 2.910200
R  4 2352.9531 6.076E+03 4.726255
R  6 2354.4338 8.164E+03 6.350329
R  8 2355.8899 9.922E+03 7.717874
R 10 2357.3212 1.129E+04 8.782356
R 12 2358.7277 1.224E+04 9.517692
R 14 2360.1095 1.275E+04 9.918749
R 16 2361.4664 1.286E+04 10.000000
R 18 2362.7985 1.259E+04 9.792624

2000, 2500
TOTAL BAND INTENSITY(GAUSSIAN SUM) = 1.8218E+05

MAXIMUM INTENSITY = 8.9935E+02
PROGRAM CO2ABS.FOR

IMPLICIT REAL*8(A-H,O-Z)
DIMENSION EL(500),EU(500),EROTP(500),EROTQ(500),
  1 EROT(500),EP(500),EQ(500),ER(500),SP(500),
  1 SQ(500),SR(500),EUQ(500)
COMMON/TBL/FRQ(1000),ST(1000),NLEV(1000)
COMMON/FREQ/FMIN,FMAX
COMMON/BINS/BINST(5000),BININDEX(5000),NBINS,WIDTH
COMMON/OUTPUT/ACCESS2$
CHARACTER*8 FILENM1$,FILENM2$
CHARACTER*24 ACCESS1$,ACCESS2$
INTEGER*2 IYEAR,IMONTH,IDAY,IHOUR,IMINUTE
CALL GETTIM(IHOUR,IMINUTE)
CALL GETDAT(IYEAR,IMONTH,IDAY)
WRITE(6,*)' ENTER INPUT FILENAME?'
READ 19,FILENM1$

FORMAT(A8)
WRITE(6,*)' ENTER OUTPUT FILENAME?'
READ 19,FILENM2$
ACCESS1$='C:\ASYMRTR\'/FILENM1$/\'.DAT'
ACCESS2$='A: '//FILENM2$/\'.DAT'
OPEN(2,FILE=ACCESS1$,ACCESS='SEQUENTIAL')
READ(2,23) ID

FORMAT(I3)
READ(2,29) BU,DU,HU

FORMAT(3E15.10)
READ(2,29) BUQ,DUQ,HUQ
READ(2,29) BL,DL,HL

FORMAT(2I4,2F10.4)
READ(2,29) FNU1,FNU2,FNU3
READ(2,49) FNUZ,FLOW,FHIGH

FORMAT(3F16.8)
READ(2,59) SV,TT

FORMAT(2F16.8)
READ(2,69) NBINS,WIDTH

FORMAT(I5,F10.6)
CLOSE(2)
WRITE(6,1019)

FORMAT(' OUTPUT FROM PROGRAM CO2ABS//')
WRITE(6,1025) IMONTH,IDAY,IYEAR
WRITE(6,1026) IHOUR,IMINUTE

FORMAT(1X,I2,'/',I2,'/',I4)

FORMAT(1X,I2,':',I2/)

WRITE(6,1029) FILENM1$

FORMAT(' INPUT FILE = ',A8/)
WRITE(6,1039) FILENM2$

FORMAT(' OUTPUT FILE = ',A8/)
WRITE(6,1024) ID

FORMAT(' ID = ',I3)
WRITE(6,1049) BU,DU,HU
1049 FORMAT( ' UPPER STATE CONSTANTS'/
1 ' B = ',F16.8,3X, 'D = ',1PE10.4,3X, 'H = ',1PE10.4/) WRITE(6,1054) BUQ,DUQ,HUQ
1054 FORMAT( ' UPPER STATE CONSTANTS (OTHER DOUBLET LEVEL)/
1 ' B = ',F16.8,3X, 'D = ',1PE10.4,3X, 'H = ',1PE10.4/) WRITE(6,1059) BL,DL,HL
1059 FORMAT( ' LOWER STATE CONSTANTS'/
1 ' B = ',F16.8,3X, 'D = ',1PE10.4,3X, 'H = ',1PE10.4/) WRITE(6,1069) JMIN,JMAX,FMIN,FMAX
1069 FORMAT( '/ J RANGE ',I4, ' TO ',I4/
1 ' FREQUENCY RANGE ',F10.4, ' TO ',F10.4/) WRITE(6,1079) FN1,FN2,FN3
1079 FORMAT( ' BAND ORIGIN ',F10.4, ' CM-1'/
1 ' NU1 ',F10.4, ' CM-1'/
2 ' NU2 ',F10.4, ' CM-1'/
3 ' NU3 ',F10.4, ' CM-1/') WRITE(6,1084) FLOW
1084 FORMAT( ' LOWER STATE VIBRATIONAL ENERGY = ',F10.4,
1 ' CM-1'/) WRITE(6,1086) FHIGH
1086 FORMAT( ' UPPER VIBRATIONAL STATE ENERGY = ',F10.4,
1 ' CM-1'/) WRITE(6,1089) SV,TT,NBINS,WIDTH
1089 FORMAT( ' BAND STRENGTH ',F16.8/
1 ' TEMPERATURE ',F10.4/
2 ' NBINS ',I5/
3 ' WIDTH ',F10.6/) C2=1.438786 NLINE=0 DO 2000 I=JMIN,JMAX EL(I)=BL*I*(I+1)-DL*(I**2)*((I+1)**2)+HL*(I**3)*((I+1)**3)
2000 CONTINUE DO 2500 I=JMIN,JMAX EU(I)=BU*I*(I+1)-DU*(I**2)*((I+1)**2)+HU*(I**3)*((I+1)**3)
2500 CONTINUE DO 2600 I=JMIN,JMAX EUQ(I)=BUQ*I*(I+1)-DUQ*(I**2)*((I+1)**2)+HUQ*(I**3)*((I+1)**3)
2600 CONTINUE DO 3000 I=JMIN+2,JMAX,2 EROTP(I)=EU(I-1)-EL(I)
3000 CONTINUE DO 3500 I=JMIN,JMAX-2,2 EROTR(I)=EU(I+1)-EL(I)
3500 CONTINUE VIBPFTO=1./((1.-DEXP(-C2*FN1/296.))*((1.-DEXP(-C2*FN2/TT))**2)*((1.-DEXP(-C2*FN3/296.)))) VIBLZMTO=DEXP(-C2*FLOW/296.) ROTPFT0=296./BL VIBLZM=DEXP(-C2*FLOW/TT)
ROTPF = TT/BL
VIBPF=1./(((1.-DEXP(-C2*FNU1/TT)))*((1.-DEXP(-C2*FNU2/TT))*((1.-DEXP(-C2*FNU3/TT)))))
S=(VIBLM*SV*VIBPT0)/(VIBLMTO*VIBPF*ROTPF)
IF(ID.LT.20) GO TO 3900
DO 3600 I=JMIN+2,JMAX-2,2
EROT(I)=EUQ(I)-EL(I)
3600 CONTINUE
DO 3700 I=JMIN+2,JMAX-2,2
FREQ=EROTQ(I)+FNUZ
ROTBLZM=DEXP((-C2*EL(I)/TT))
STIMEM=(1.-DEXP((-C2*FREQ)/TT))
IF(ID.EQ.22) THEN
HLFAC=(2.*REAL(I)+1.)/4.
ELSE
HLFAC=(2.*REAL(I)+1.)/((REAL(I)) *(REAL(I)+1.))
ENDIF
SQ(I)=S*FREQ*HLFAC*STIMEM*ROTBLZM/FNUZ
STRE=SQ(I)
NTYPE=2000+I
IF(FREQ.GE.FMIN.AND.FREQ.LE.FMAX) THEN
CALL STORE(NLINE,FREQ,STRE,NTYPE)
ENDIF
3700 CONTINUE
SMAX=0.000001
DO 4000 I=JMIN+2,JMAX,2
FREQ=EROTP(I)+FNUZ
ROTBLZM=DEXP((-C2*EL(I)/TT))
STIMEM=(1.-DEXP((-C2*FREQ)/TT))
IF(ID.EQ.11) THEN
HLFAC=REAL(I)
ELSEIF(ID.EQ.22) THEN
HLFAC=REAL(I)*(REAL(I)-1)/(4.*REAL(I))
ELSE
HLFAC=(REAL(I)+1.)*(REAL(I)-1.)/REAL(I)
ENDIF
SP(I)=S*FREQ*HLFAC*STIMEM*ROTBLZM/FNUZ
STRE=SP(I)
NTYPE=1000+I
IF(FREQ.GE.FMIN.AND.FREQ.LE.FMAX) THEN
CALL STORE(NLINE,FREQ,STRE,NTYPE)
ENDIF
4000 CONTINUE
DO 5000 I=JMIN,JMAX-2,2
FREQ=EROTR(I)+FNUZ
ROTBLZM=DEXP((-C2*EL(I)/TT))
STIMEM=(1.-DEXP((-C2*FREQ)/TT))
IF(ID.EQ.11) THEN
HLFAC=REAL(I)+1.
ELSEIF(ID.EQ.22) THEN
HLFAC=(REAL(I)+2.)/4.
ELSE
HLFAC=(REAL(I)+2.)*REAL(I)/(REAL(I)+1.)
ENDIF
SR(I) = S * FREQ * HLFAC * STIMEM * ROTBL2M / FNUZ
STRE = SR(I)
NTYPE = 3000 + I
IF (FREQ .GE. FMIN .AND. FREQ .LE. FMAX) THEN
CALL STORE (NLINE, FREQ, STRE, NTYPE)
ENDIF
5000 CONTINUE
CALL SORT (NLINE)
CALL PRINT (NLINE)
CALL BINSORT (NLINE)
CALL SHAPE (NLINE)
STOP
END
C

PROGRAM CO2EMS FOR

IMPLICIT REAL*8(A-H,O-Z)

DIMENSION EL(500), EU(500), EROTP(500), EROTQ(500),
1 EROT(500), EP(500), EQ(500), ER(500), SP(500),
2 SQ(500), SR(500), EUQ(500)

COMMON/TBL/FRQ(1000), ST(1000), NLEV(1000)
COMMON/FREQ/FMIN, FMAX
COMMON/BINS/BINST(5000), BINDEX(5000), NBINS, WIDTH
COMMON/OUTPUT/ACCESS2$

CHARACTER*8 FILENM1$, FILENM2$
CHARACTER*24 ACCESS1$, ACCESS2$

INTEGER*2 IYEAR, IMONTH, IDAY, IHOUR, IMINUTE

CALL GETTIM(IHOUR, IMINUTE)

CALL GETDAT(IYEAR, IMONTH, IDAY)

WRITE(6,*)

ENTER INPUT FILENAME?

READ 19, FILENM1$

19 FORMAT(A8)

WRITE(6,*)

ENTER OUTPUT FILENAME?

READ 19, FILENM2$

ACCESS1$='C:\ASYMRTR'//FILENM1$//' .DAT'

ACCESS2$='A:'//FILENM2$//' .DAT'

OPEN(2, FILE=ACCESS1$, ACCESS='SEQUENTIAL')

READ(2,23) ID

23 FORMAT(I3)

READ(2,29) BU, DU, HU

29 FORMAT(3E15.10)

READ(2,29) BUQ, DUQ, HUQ

READ(2,29) BL, DL, HL

READ(2,39) JMIN, JMAX, FMIN, FMAX

39 FORMAT(2I4,2F10.4)

READ(2,29) FNU1, FNU2, FNU3

49 FORMAT(3F16.8)

READ(2,59) SV, TT

59 FORMAT(2F16.8)

READ(2,69) NBINS, WIDTH

69 FORMAT(I5,F10.6)

CLOSE(2)

WRITE(6,1019)

1019 FORMAT('OUTPUT FROM PROGRAM CO2EMS')/

WRITE(6,1025) IMONTH, IDAY, IYEAR

WRITE(6,1026) IHOUR, IMINUTE

1025 FORMAT(1X,I2, '/',I2,'/',I4)

1026 FORMAT(1X,I2,':',I2/)

WRITE(6,1029) FILENM1$

1029 FORMAT('INPUT FILE = ',A8)

WRITE(6,1039) FILENM2$

1039 FORMAT('OUTPUT FILE = ',A8)

WRITE(6,1024) ID

1049 FORMAT('UPPER STATE CONSTANTS'/
1 ' B = ',F16.8,3X,'D = ',1PE10.4,3X,'H = ',1PE10.4)
WRITE(6,1054) BUQ,DUQ,HUQ
1054 FORMAT(' UPPER STATE CONSTANTS(OTHER DOUBLET LEVEL)/'
1 ' B = ',F16.8,3X,'D = ',1PE10.4,3X,'H = ',1PE10.4/
WRITE(6,1059) BL,DL,HL
1059 FORMAT(' LOWER STATE CONSTANTS'/
1 ' B = ',F16.8,3X,'D = ',1PE10.4,3X,'H = ',1PE10.4/
WRITE(6,1069) JMIN,JMAX,FMIN,FMAX
1069 FORMAT(' J RANGE ','I4,' TO ','I4/
1 ' FREQUENCY RANGE ','F10.4,' TO ','F10.4/
WRITE(6,1079) FN1,FN2,FN3
1079 FORMAT(' BAND ORIGIN ','F10.4,' CM-1/
1 ' NU1 ','F10.4,' CM-1/
2 ' NU2 ','F10.4,' CM-1/
3 ' NU3 ','F10.4,' CM-1/
WRITE(6,1084) FLOW
1084 FORMAT(' LOWER VIBRATIONAL STATE ENERGY = ','F10.4,' CM-1/
WRITE(6,1086) FHIGH
1086 FORMAT(' UPPER VIBRATIONAL STATE ENERGY = ','F10.4,' CM-1/
WRITE(6,1089) SV,TT,NBINS,WIDTH
1089 FORMAT(' BAND STRENGTH ','F16.8/
1 ' TEMPERATURE ','F10.4/
2 ' NBINS ','I5/
3 ' WIDTH ','F10.6///)

C2=1.438786
NLIN=0
DO 2000 I=JMIN,JMAX
2000 CONTINUE
EL(I)=BL*I*(I+1)-DL*(I**2)*((I+1)**2)+HL*(I**3)*
1((I+1)**3)
DO 2500 I=JMIN,JMAX
2500 CONTINUE
EU(I)=BU*I*(I+1)-DU*(I**2)*((I+1)**2)+HU*(I**3)*
1((I+1)**3)
DO 2600 I=JMIN,JMAX
2600 CONTINUE
EUQ(I)=BUQ*I*(I+1)-DUQ*(I**2)*((I+1)**2)+HUQ*(I**3)*
1((I+1)**3)
DO 3000 I=JMIN+2,JMAX,2
3000 CONTINUE
EROTP(I)=EU(I-1)-EL(I)
DO 3500 I=JMIN,JMAX-2,2
3500 CONTINUE
EROTR(I)=EU(I+1)-EL(I)
DO 3700 I=JMIN,JMAX
3700 CONTINUE
VIBPFT0=1./((1.-DEXP(-C2*FN1/296.))*((1.-DEXP
1 (-C2*FN2/296.))*2)*(1.-DEXP(-C2*FN3/296.))))
VIBLZMT0=DEXP(-C2*FLOW/296.)
ROTP0=296./BL
VIBLZM=DEXP(-C2*FHIGH/TT)
ROTPF=TT/BL
VIBPF=1./((1.-DEXP(-C2*FN1/TT))*((1.-DEXP
1 (-C2*FN2/TT))*2)*(1.-DEXP(-C2*FN3/TT))))
\[ S = \frac{(VIBZM \cdot SV \cdot VIBPFT0)}{(VIBZMTO \cdot VIBPF \cdot ROTP)} \]

IF (ID.LT.20) GO TO 3900

DO 3600 I=JMIN+2,JMAX-2,2

EROTQ(I) = EUQ(I) - EL(I)

3600 CONTINUE

DO 3700 I=JMIN+2,JMAX-2,2

FREQ = EROTP(I) + FNUZ

ROTBLZM = DEXP\((-C2 \cdot EL(I))/TT)\)

C STIMEM = \(1. - DEXP((-C2 \cdot FREQ)/TT))\)

IF (ID.EQ.22) THEN

HLFAC = \((2. \cdot \text{REAL}(I)+1.)/4.\)

ELSE

HLFAC = \((2. \cdot \text{REAL}(I)+1.)/((\text{REAL}(I)) \cdot (\text{REAL}(I)+1.))\)

ENDIF

SQ(I) = \(S \cdot \text{FREQ}^X \cdot \text{HLFAC} \cdot \text{ROTBLZM} / \text{FNUZ}\)

STRE = SQ(I)

NTYPE = 2000+I

CALL STORE(NLINE, FREQ, STRE, NTYPE)

3700 CONTINUE

3900 SMAX = 0.000001

DO 4000 I=JMIN+2,JMAX,2

FREQ = EROTR(I) + FNUZ

ROTBLZM = DEXP\((-C2 \cdot EL(I))/TT)\)

C STIMEM = \(1. - DEXP((-C2 \cdot FREQ)/TT))\)

IF (ID.EQ.11) THEN

HLFAC = \(\text{REAL}(I)\)

ELSEIF (ID.EQ.22) THEN

HLFAC = \(\frac{(\text{REAL}(I) + 1.) \cdot (\text{REAL}(I) - 1)}{\text{REAL}(I)}\)

ELSE

HLFAC = \(\frac{\text{REAL}(I) + 2.}{4.}\)

ENDIF

SP(I) = \(S \cdot \text{FREQ}^X \cdot \text{HLFAC} \cdot \text{ROTBLZM} / \text{FNUZ}\)

STRE = SP(I)

NTYPE = 1000+I

CALL STORE(NLINE, FREQ, STRE, NTYPE)

4000 CONTINUE

DO 5000 I=JMIN,JMAX-2,2

FREQ = EROTR(I) + FNUZ

ROTBLZM = DEXP\((-C2 \cdot EL(I))/TT)\)

C STIMEM = \(1. - DEXP((-C2 \cdot FREQ)/TT))\)

IF (ID.EQ.11) THEN

HLFAC = \(\text{REAL}(I)+1.\)

ELSEIF (ID.EQ.22) THEN

HLFAC = \(\frac{(\text{REAL}(I) + 2.)}{4.}\)

ELSE

HLFAC = \(\frac{(\text{REAL}(I) + 2.) \cdot \text{REAL}(I)}{(\text{REAL}(I)+1.)}\)

ENDIF

SR(I) = \(S \cdot \text{FREQ}^X \cdot \text{HLFAC} \cdot \text{ROTBLZM} / \text{FNUZ}\)

STRE = SR(I)

NTYPE = 3000+I

CALL STORE(NLINE, FREQ, STRE, NTYPE)

5000 CONTINUE

CALL SORT(NLINE)
CALL PRINT(NLINE)
CALL BINSORT(NLINE)
CALL SHAPE(NLINE)
STOP
END
PROGRAM HCLEMS
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION EL(1000),EU(1000),EROTP(1000),EROTR(1000),EP(1000),ER(1000),SP(1000),SR(1000)
COMMON/TBL/FRQ(10000),ST(10000)
COMMON/FREQ/FMIN,FMAX
COMMON/BINS/BINST(5000),BINDEX(5000),NBINS,WIDTH
COMMON/OUTPUT/ACCESS2$
COMMON/INTEN/TOTINT,STRENGTH
CHARACTER*8 FILENM1$,FILENM2$
CHARACTER*24 ACCESS1$,ACCESS2$
WRITE(6,*)
ENTER INPUT FILENAME?'
READ 19,FILENM1$
 FORMAT(A8)
WRITE(6,*) ' ENTER OUTPUT FILENAME?'
READ 19, FILENM2$
ACCESS1$='C:\ASYMTR\'/FILENM1$'/'.DAT'
ACCESS2$='A: '//FILENM2$'/'.DAT'
OPEN(2,FILE=ACCESS1$,ACCESS='SEQUENTIAL')
READ(2,29) BU,DU,HU
 FORMAT(3F16.10)
READ(2,29) BL,DL,HL
READ(2,39) JMIN,JMAX,FMIN,FMAX
 FORMAT(2I4,2F10.4)
READ(2,49) FNUZ
 FORMAT(F16.8)
READ(2,59) SV,TT
 FORMAT(2F16.8)
READ(2,69) NBINS,WIDTH
 FORMAT(I5,F10.6)
CLOSE(2)
WRITE(6,1019)
 FORMAT(' OUTPUT FROM PROGRAM HCL'/)
WRITE(6,1029) FILENM1$
 FORMAT(' INPUT FILE = ',A8)
WRITE(6,1039) FILENM2$
 FORMAT(' OUTPUT FILE = ',A8)
WRITE(6,1049) BU,DU,HU
 FORMAT(' UPPER STATE CONSTANTS'/
 ' B = ',F16.8,'D = ',F16.8,'H = ',F16.8/)
WRITE(6,1059) BL,DL,HL
 FORMAT(' LOWER STATE CONSTANTS'/
 ' B = ',F16.8,'D = ',F16.8,'H = ',F16.8/)
WRITE(6,1069) JMIN,JMAX,FMIN,FMAX
 FORMAT(' J RANGE ',I4,' TO ',I4/
 ' FREQUENCY RANGE ',F10.4,' TO ',F10.4/)
WRITE(6,1079) FNUZ
 FORMAT(' BAND ORIGIN ',F10.4,' CM-1'/)
WRITE(6,1089) SV,TT,NBINS,WIDTH
 FORMAT(' BAND STRENGTH ',F16.8/
 ' TEMPERATURE ',F10.4/
 ' NBINS ',I5/
 ' WIDTH ',F10.6//)
C2=1.438786
NLINE=0
TOTINT=0.0
DO 2000 I=JMIN,JMAX
   EL(I)=BL*I*(I+1)-DL*(I**2)*((I+1)**2)+HL*(I**3)(I+1)**3
1100 FORMAT(' J=',I4,' ER=',F10.4)
2000 CONTINUE
DO 2500 I=JMIN,JMAX
   EU(I)=BU*I*(I+1)-DU*(I**2)*((I+1)**2)+HU*(I**3)(I+1)**3
2500 CONTINUE
DO 3000 I=JMIN,JMAX
   EROTP(I)=EU(I-1)-EL(I)
3000 CONTINUE
DO 3500 I=JMIN+1,JMAX
   EROTR(I)=EU(I+1)-EL(I)
3500 CONTINUE
VIBPFT0=1./((1.-DEXP(-C2*FNUZ/296.))
VIBLZMTO=DEXP(-C2*FNUZ/296.)
ROTPF0=296./BL
VIBLM=DEXP(-C2*FNUZ/TT)
ROTPF=TT/BL
VIBPF=1./((1.-DEXP(-C2*FNUZ/TT))
SMAX=0.0001
DO 4000 I=JMIN+1,JMAX
   FREQ=EROTP(I)+FNUZ
   ROTBLZM=DEXP((-C2*EU(I))/TT)
   HLFAC=I
   MM=-I
   FF=1.+(-2.5599E-2)*MM+(3.203E-4)*MM**2
   STRENGTH=HLFAC*ROTBLZM/ROTPF
   SP(I)=FREQ**4*VIBLZM*VIBPFT0*FF*STRENGTH/
      (FNUZ*VIBPF)
   IF(SP(I).GT.SMAX) SMAX=SP(I)
   EP(I)=FREQ
   STRE=SP(I)
1099 FORMAT(' P ',3X,I4,5X,F10.4,5X,1PE9.3,5X,F10.6)
   IF(FREQ.GE.FMIN.AND.FREQ.LE.FMAX) THEN
      CALL STORE(NLINE,FREQ,STRE)
   ENDIF
4000 CONTINUE
DO 5000 I=JMIN,JMAX-1
   FREQ=EROTR(I)+FNUZ
   ROTBLZM=DEXP((-C2*EU(I))/TT)
   HLFAC=I+1.
   MM=I+1.
   FF=1.+(-2.5599E-2)*MM+(3.203E-4)*MM**2
   STRENGTH=HLFAC*ROTBLZM/ROTPF
   SR(I)=FREQ**4*VIBLZM*VIBPFT0*FF*STRENGTH/
      (FNUZ*VIBPF)
   IF(SR(I).GT.SMAX) SMAX=SR(I)
   ER(I)=FREQ
69
STRE = SR(I)
IF (FREQ.GE.FMIN.AND.FREQ.LE.FMAX) THEN
CALL STORE(NLINE,FREQ,STRE)
ENDIF
5000 CONTINUE
DO 6000 I = JMAX,JMIN+1,-1
SREL = SP(I)/SMAX
WRITE(6,1099) I,EP(I),SP(I),SREL
6000 CONTINUE
DO 7000 I = JMIN,JMAX-1
SREL = SR(I)/SMAX
WRITE(6,1109) I,ER(I),SR(I),SREL
1109 FORMAT(' R ',3X,I4,5X,F10.4,5X,1PE9.3,5X,F10.6)
7000 CONTINUE
WRITE(6,1119) TOTINT
1119 FORMAT(' TOTINT = ',F10.6)
CALL SORT(NLINE)
CALL BINSORT(NLINE)
CALL SHAPE(NLINE)
STOP
END
Table 1 - Statistical Weight Factors for Isotopes of Water

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Value of</th>
<th>Symmetry</th>
<th>Relative Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>H$_2$O</td>
<td>odd</td>
<td>antisymmetric</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>even</td>
<td>symmetric</td>
<td>1</td>
</tr>
<tr>
<td>D$_2$O</td>
<td>odd</td>
<td>antisymmetric</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>even</td>
<td>symmetric</td>
<td>6</td>
</tr>
<tr>
<td>HDO</td>
<td>odd or even</td>
<td>no identical nuclei</td>
<td>1</td>
</tr>
</tbody>
</table>
Table 2 - Hönli-London Factors for CO$_2$

<table>
<thead>
<tr>
<th>$\Delta \ell = 0$</th>
<th>$\Delta \ell = 0$</th>
<th>$\Delta \ell = 0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Sigma - \Sigma ) bands</td>
<td>( J )</td>
<td>( - )</td>
</tr>
<tr>
<td>( \Pi - \Pi ) bands</td>
<td>( \frac{(J+1)(J-1)}{J} )</td>
<td>( \frac{(J+1)}{J(J+1)} )</td>
</tr>
<tr>
<td>$\Delta \ell = 1$</td>
<td>$\Delta \ell = 1$</td>
<td>$\Delta \ell = 1$</td>
</tr>
<tr>
<td>( \Pi - \Sigma ) bands</td>
<td>( \frac{J(J-1)}{4J} )</td>
<td>( \frac{J+1}{4} )</td>
</tr>
</tbody>
</table>
Table 3 - Constants for H₂O Calculations

Rotational Constants (in cm⁻¹)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>27.88067</td>
<td>27.12217</td>
<td>31.1283₂</td>
<td>26.6480₅</td>
<td>35.586₇₂</td>
</tr>
<tr>
<td>Δₖ x 10³</td>
<td>1.24₈₉₄</td>
<td>1.2₃₃₀</td>
<td>1.₃₉₅₇</td>
<td>1.₃₀₅₄</td>
<td>1.₅₈₀₄</td>
</tr>
<tr>
<td>Δₖ x 10³</td>
<td>-5.₇₆₅₅</td>
<td>-5.₃₇₄₇</td>
<td>-7.₆₀₅₃</td>
<td>-5.₆₅₆₁</td>
<td>-10.₄₈₄</td>
</tr>
<tr>
<td>Δₖ x 10²</td>
<td>3.₂₅₁₉₉</td>
<td>3.₀₂₃₀</td>
<td>5.₇₅₅₀₄</td>
<td>2.₈₅₈₄</td>
<td>10.₉₉₁₉</td>
</tr>
<tr>
<td>δₖ x 10⁴</td>
<td>5.₀₈₃₈</td>
<td>4.₉₉₈₇</td>
<td>5.₇₈₇₉</td>
<td>5.₃₁₇</td>
<td>6.₇₅₂</td>
</tr>
<tr>
<td>δₖ x 10³</td>
<td>1.₃₀₀₇</td>
<td>1.₂₄₀₅</td>
<td>3.₇₆₆₂</td>
<td>1.₃₂₆</td>
<td>8.₇₁₃</td>
</tr>
</tbody>
</table>

Vibrational Constants[8]

<table>
<thead>
<tr>
<th>ν'</th>
<th>ν''</th>
<th>ν₀(cm⁻¹)</th>
<th>S₀ x 10²₀(cm molecule)</th>
<th>Band Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1₀₀</td>
<td>0₀₀</td>
<td>3₆₅₇.₀₅₅</td>
<td>4₈.₆₂</td>
<td>B</td>
</tr>
<tr>
<td>0₁₀</td>
<td>0₀₀</td>
<td>1₅₉₄.₇₇₈</td>
<td>1₀₃₈.₀</td>
<td>B</td>
</tr>
<tr>
<td>0₀₁</td>
<td>0₀₀</td>
<td>3₇₅₅.₉₃₀</td>
<td>6₉₂.₅</td>
<td>A</td>
</tr>
<tr>
<td>0₂₀</td>
<td>0₀₀</td>
<td>3₁₅₁.₆₃₀</td>
<td>7.₅₃₇</td>
<td>B</td>
</tr>
</tbody>
</table>
Table 4 - Constants for D$_2$O Calculation

Rotational Constants

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$ (cm$^{-1}$)</td>
<td>15.3846</td>
<td>15.1286</td>
<td>16.6338802</td>
<td>14.7916</td>
</tr>
<tr>
<td>$B$ (cm$^{-1}$)</td>
<td>7.2716</td>
<td>7.1696</td>
<td>7.3388231</td>
<td>7.2266</td>
</tr>
<tr>
<td>$C$ (cm$^{-1}$)</td>
<td>4.8458</td>
<td>4.7698</td>
<td>4.7894858</td>
<td>4.7908</td>
</tr>
</tbody>
</table>

Vibrational Constants

<table>
<thead>
<tr>
<th>$v'$</th>
<th>$v''$</th>
<th>$\nu_0$ (cm$^{-1}$)[13]</th>
<th>$S_0 \times 10^{20}$ (cm molecule)$^{-1}$</th>
<th>Band Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>000</td>
<td>2672.0811</td>
<td>54.0</td>
<td>B</td>
</tr>
<tr>
<td>010</td>
<td>000</td>
<td>1178.374</td>
<td>564.</td>
<td>B</td>
</tr>
<tr>
<td>001</td>
<td>000</td>
<td>2787.7182</td>
<td>486.</td>
<td>A</td>
</tr>
</tbody>
</table>
### Table 5 - Constants for HDO Calculation

#### Rotational Constants

<table>
<thead>
<tr>
<th>(v_1)</th>
<th>(v_2)</th>
<th>(v_3)</th>
<th>Rotational Constants</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>A(cm(^{-1}))</th>
<th>B(cm(^{-1}))</th>
<th>C(cm(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>23.413842</td>
<td>9.103323</td>
<td>6.406295</td>
</tr>
<tr>
<td>23.095854</td>
<td>8.925215</td>
<td>6.3042430</td>
</tr>
<tr>
<td>25.551</td>
<td>9.238</td>
<td>6.335</td>
</tr>
<tr>
<td>22.3226</td>
<td>9.0850</td>
<td>6.3293</td>
</tr>
<tr>
<td>28.255498</td>
<td>9.367797</td>
<td>6.2400774</td>
</tr>
</tbody>
</table>

#### Vibrational Constants

<table>
<thead>
<tr>
<th>(v')</th>
<th>(v'')</th>
<th>(\nu_0(cm^{-1})[15])</th>
<th>(S\times10^{20}(cm/molecule))</th>
<th>Band Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>000</td>
<td>2723.680</td>
<td>215. [18]</td>
<td>A</td>
</tr>
<tr>
<td>100</td>
<td>000</td>
<td>2723.680</td>
<td>1.73 [18]</td>
<td>B</td>
</tr>
<tr>
<td>010</td>
<td>000</td>
<td>1403.421</td>
<td>406.2 [19]</td>
<td>A</td>
</tr>
<tr>
<td>010</td>
<td>000</td>
<td>1403.421</td>
<td>532.8 [19]</td>
<td>B</td>
</tr>
<tr>
<td>001</td>
<td>000</td>
<td>3707.47</td>
<td>350.3 [20]</td>
<td>A</td>
</tr>
<tr>
<td>001</td>
<td>000</td>
<td>3707.47</td>
<td>145.3 [20]</td>
<td>B</td>
</tr>
<tr>
<td>020</td>
<td>000</td>
<td>2782.012</td>
<td>24.2 [18]</td>
<td>A</td>
</tr>
<tr>
<td>020</td>
<td>000</td>
<td>2782.012</td>
<td>11.1 [18]</td>
<td>B</td>
</tr>
</tbody>
</table>
Table 6 - Constants for CO₂ Calculation

Rotational Constants[7]

<table>
<thead>
<tr>
<th>ν*</th>
<th>Cₜ(cm⁻¹)</th>
<th>B(cm⁻¹)</th>
<th>Dₓ10⁻⁷(cm⁻¹)</th>
<th>Hₓ10⁻¹³(cm⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>00001</td>
<td>0.</td>
<td>0.39021817</td>
<td>1.33204</td>
<td>0.055</td>
</tr>
<tr>
<td>01101 e</td>
<td>667.3801</td>
<td>0.39063825</td>
<td>1.35133</td>
<td></td>
</tr>
<tr>
<td>01101 f</td>
<td>667.3801</td>
<td>0.39125388</td>
<td>1.35900</td>
<td></td>
</tr>
<tr>
<td>00011</td>
<td>2349.1433</td>
<td>0.38714069</td>
<td>1.32873</td>
<td>0.077</td>
</tr>
<tr>
<td>01111 e</td>
<td>3004.0122</td>
<td>0.38759172</td>
<td>1.34546</td>
<td></td>
</tr>
<tr>
<td>01111 f</td>
<td>3004.0122</td>
<td>0.38818943</td>
<td>1.35522</td>
<td></td>
</tr>
<tr>
<td>10012</td>
<td>3612.8417</td>
<td>0.38750237</td>
<td>1.57314</td>
<td>2.024</td>
</tr>
<tr>
<td>10011</td>
<td>3714.7828</td>
<td>0.38706251</td>
<td>1.14177</td>
<td>1.989</td>
</tr>
</tbody>
</table>

*For band notation, see[3], pp. 23-24

Vibrational Constants[7]

<table>
<thead>
<tr>
<th>ν₀(cm⁻¹)</th>
<th>ν'</th>
<th>ν''</th>
<th>S₀x10²⁰(cm/molecule)</th>
<th>Band Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>667.380</td>
<td>01101</td>
<td>00001</td>
<td>82580.</td>
<td>Πᵤ - Σ⁺_g</td>
</tr>
<tr>
<td>2356.632</td>
<td>01111</td>
<td>01101</td>
<td>73700.</td>
<td>Πₕ - Πᵤ</td>
</tr>
<tr>
<td>2349.143</td>
<td>00011</td>
<td>00001</td>
<td>955900.</td>
<td>Σ⁺ₕ - Σ⁺ₕ</td>
</tr>
<tr>
<td>3612.842</td>
<td>10012</td>
<td>00001</td>
<td>10400.</td>
<td>Σ⁺ₕ - Σ⁺ₕ</td>
</tr>
<tr>
<td>3714.783</td>
<td>10011</td>
<td>00001</td>
<td>15800.</td>
<td>Σ⁺ᵤ - Σ⁺ₕ</td>
</tr>
</tbody>
</table>

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Table 7 - Constants for HCℓ Calculations

Rotational Constants[24]

<table>
<thead>
<tr>
<th></th>
<th>B(cm(^{-1}))</th>
<th>D(cm(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>H(^{35})Cℓ(v=0)</td>
<td>10.4400</td>
<td>0.000530</td>
</tr>
<tr>
<td>H(^{35})Cℓ(v=1)</td>
<td>10.1381</td>
<td>0.000526</td>
</tr>
<tr>
<td>D(^{35})Cℓ(v=0)</td>
<td>5.392149</td>
<td>0.0001397</td>
</tr>
<tr>
<td>D(^{35})Cℓ(v=1)</td>
<td>5.278858</td>
<td>0.0001410</td>
</tr>
</tbody>
</table>

Vibrational Constants[24]

<table>
<thead>
<tr>
<th></th>
<th>(\nu_0)(cm(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>H(^{35})Cℓ</td>
<td>2885.82</td>
</tr>
<tr>
<td>D(^{35})Cℓ</td>
<td>2091.079</td>
</tr>
</tbody>
</table>
Fig. 1 - Simulated absorption spectra of H$_2$O at 296K, 1000K, and 1730K.
Fig. 2 - Simulated emission spectra of $\text{D}_2\text{O}$, HDO and $\text{H}_2\text{O}$ at 1750K.
Fig. 3 - Simulated emission spectrum of an equimolar H$_2$O-D$_2$O mixture at 1730K.
Fig. 4 - Simulated absorption spectra of CO$_2$ at 296K, 1000K, and 1730K.
Fig. 5 - Simulated emission spectra of CO$_2$ at 1000K and 1730K
Fig. 6 - Simulation of hot CO₂ emission spectrum at 1730K, cold CO₂ absorption spectrum at 296K, and hot CO₂ emission viewed through absorbing cold CO₂.
Fig. 7 - Simulated emission spectra of HCl and DCl at 1730K.
END
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