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Quadrupole $N_2$ lines at 4.1 $\mu$m studied with a diode laser and an absorption path of 5.016 km

Balog, Paul P., Ph.D.
The Ohio State University, 1990
QUADRUPOLE $N_2$ LINES AT 4.1 $\mu$m
STUDIED WITH A DIODE LASER AND
AN ABSORPTION PATH OF 5.016 km

DISSERTATION
Presented in Partial Fulfillment of the Requirements
for the Degree Doctor of Philosophy in the Graduate
School of The Ohio State University

By
Paul P. Balog, B.S., M.S.

* * * * *

The Ohio State University
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CHAPTER I
INTRODUCTION

1.1 Motivation for the Study of \( \text{N}_2 \) Quadrupole Transitions

In 1938, Herzberg\(^1\) published a paper entitled "On the Possibility of Detecting Molecular Hydrogen and Nitrogen in Planetary and Stellar Atmospheres by their Rotation-Vibration Spectra." In this paper and in a companion paper in the same journal by James and Coolidge\(^2\), it was suggested that \( \text{N}_2 \) could be detected via its quadrupole rotation-vibration spectrum in the atmosphere of planets or cool stars, where the great depth of the absorbing material, i.e., \( \text{H}_2 \) or \( \text{N}_2 \), could compensate for the small absorption coefficient. In fact, Herzberg computed that the minimum absorbing layer required to detect the 1-0 band of \( \text{H}_2 \) was 2.5 km-atm, and stated that the detection of the \( \text{N}_2 \) bands will probably be more difficult than the detection of the \( \text{H}_2 \) bands. The difficulty with measuring absorption spectra from either \( \text{H}_2 \) or \( \text{N}_2 \) is that neither have a permanent dipole moment. The existence of infrared rotation-vibration spectra for the majority of molecules is due to the molecule's dipole moment. Intense sources of radiation, extremely long absorbing paths, high pressures, or some combination of these are needed to observe quadrupole transitions.

The first detection of a quadrupole spectrum did not occur until 1949, as reported by Herzberg\(^3,4\). Four lines in each the 2-0 and 3-0
bands of the quadrupole spectrum of H\textsubscript{2} were detected in the laboratory using effective optical densities (absorbing path times gas pressure) of 10 to 50 km-atm. The first extraterrestrial detection of a quadrupole spectrum (H\textsubscript{2}) did not occur until 1960\textsuperscript{6} with the detection of four lines of the 3-0 band of H\textsubscript{2} in the spectra of Jupiter.

The pure rotational Raman spectra of N\textsubscript{2} was studied by Stoicheff\textsuperscript{6} in 1954, and Butcher et al.\textsuperscript{7} in 1971, and Bendtsen\textsuperscript{8} in 1974. From these studies, values for the molecular constants B\textsubscript{e} and r\textsubscript{e} were obtained. Bendtsen also studied the rotational-vibrational Raman spectra of N\textsubscript{2}, from which the positions of the 0, Q, and S lines of the fundamental vibrational band could be determined.

The first direct observation of N\textsubscript{2} quadrupole lines was by Camy-Peyret et al.\textsuperscript{9} in 1981 using the sun as the source, and the intervening atmosphere as the sample under investigation. Using the 1-m Fourier transform spectrometer, located at the Kitt Peak National Observatory, with a resolution of 0.009 cm\textsuperscript{-1}, they were able to observe the S(7) through S(16) lines of the 1-0 band of N\textsubscript{2}. An effective optical density of 5 km-atm was computed for these measurements. More recently and as shown\textsuperscript{10} in figure 1, are spectra containing the S(10) and S(12) quadrupole absorption lines of N\textsubscript{2}. The ATMOS (Atmospheric Trace Molecule Spectroscopy experiment) was included as part of the Spacelab 3 payload which flew on the shuttle "Challenger" in May, 1985. These spectra were recorded in a limb view of the atmosphere, with the Sun as the source, with the tangent height noted in kilometers along the right. The shuttle was at an altitude, Z, of 360 km. The ATMOS ground-based measurements were taken five months later at the Table Mountain Observatory in the San Gabriel
Figure 1. $N_2$ (1-0) Quadrupole Transitions - Atmospheric Spectra
Mountains north of Los Angeles. The angle $\theta$ is the solar zenith angle for these observations. Finally, Jungfraujoch refers to the Fourier transform spectrometer located on the Jungfraujoch mountain in Switzerland. Measurements were made at this facility by a Belgian group (Liege) under contract to the Jet Propulsion Laboratory in Pasadena, California.

One of the objectives of the ATMOS project was to determine the vertical mixing ratio profiles in the upper atmosphere of certain minor and trace constituents, such as CFCl$_3$, CF$_2$Cl$_2$, CCl$_4$, N$_2$O, and H$_2$O. This objective was motivated, at least in part, by the concern over anthropogenically induced modifications to the Earth's ozone layer. In order to obtain these profiles from the ATMOS data, the temperature and pressure profile over the relevant region of the atmosphere must first be determined. Spectral features are present in the ATMOS data that can be used to extract these quantities from a number of the individual occultations. Lines from several ground-state transition bands of CO$_2$ can be used to determine pressure and temperature over altitudes from 20 km to approximately 70 km, and, by virtue of their insensitivity to temperature, the S(8) and S(10) lines from the N$_2$ 1-0 quadrupole band, which have lower state energies on the order of 200 cm$^{-1}$, can also be used to retrieve the line of sight column density from 20 to 35 km. Since tangent ray paths in this region correspond to airmass values between approximately 10 and 1, the N$_2$ lines can be carefully "calibrated" to indicate the tangent height by reference to spectral scans made by the instrument observing the Sun from the ground at equivalent airmasses.$^{11}$

The first and only laboratory measurements to date of quadrupole transitions in N$_2$ was reported by Reuter et al.$^{12}$ in 1986. Using the Kitt
Peak Fourier transform spectrometer, transitions in the O and S branches of the \( \nu = 1 \rightarrow 0 \) band of \( \text{N}_2 \) were observed. In this case, a White\textsuperscript{13} cell with the path length adjusted to 434 m and pressures of 249, 605, and 1580 Torr was used as the absorbing medium. The resolutions for each of these pressures were 0.010, 0.025, and 0.050 cm\(^{-1}\), respectively. This is equivalent to optical densities ranging from 0.142 to 0.902 km-atm. Measurements with these lower optical densities were possible because hundreds of scans, recorded over periods of from 4.5 to 8.5 hours, were averaged together. The half-widths of the S(10) and S(12) lines of \( \text{N}_2 \) were reported to be 0.0286 and 0.0309 cm\(^{-1}\) at 605 Torr. In order to accurately measure the half-width, the experiment needs to be conducted under controlled laboratory conditions, as was done in this case, and the resolution of the spectrometer should be significantly finer than the half-width to be measured.

In the present work a high resolution laser diode spectrometer and a 22 m base-length White cell were used to characterize the S(8), S(10), and S(12) quadrupole lines of \( \text{N}_2 \) with optical densities ranging from 4.81 to 6.27 km-atm. The diode laser had an ultimate resolution limit (Doppler width) of 0.0003 cm\(^{-1}\). The experiment was conducted by stepping the laser in increments of 0.0015 cm\(^{-1}\), which was found to be both sufficient for the characterization of the line and practical with respect to the time required per scan. These data were obtained after relocating the Spectroscopy Facility from the National Oceanic and Atmospheric Administration (NOAA) in Suitland, Maryland to The Ohio State University in Columbus, Ohio. A portion of this equipment was then relocated to Denison University in Granville, Ohio in order to achieve the path length of 5.016
km possible with the 22 m White cell there.

1.2 Overview

Some of the equipment obtained from NOAA had never been put into function. In particular, a 4 m stainless-steel White cell had been built at NOAA and generally leak-tested. However there were no remote controls available for the mirrors, and one of the entry windows was incorrectly placed.

After the equipment was made to be functional and the appropriate calibrations had been performed, attempts to observe lines in the quadrupole spectrum of N$_2$ were made using the 4 m stainless-steel White cell mentioned above adjusted to a path length of 408 m. Unable to detect the weak absorption lines, considerable effort went into preparing a 10 m White cell for the same task. After taking some preliminary signal-to-noise ratio measurements, all of which were unacceptably low, with the 10 m cell set to approximately 1.4 km, the laser diode spectrometer was moved to Denison University to couple it with the 22 m fiberglass White cell in order to increase the absorption path beyond 1.4 km.

After correcting several additional equipment malfunctions which occurred after moving the spectrometer to Denison, the S(8), S(10), and S(12) lines of N$_2$ were detected using second derivative spectroscopy. The low signal to noise ratio in the S(8) region precluded any characterization of that line. This was due entirely to the low output of the laser at that wavelength. However, the S(10) and S(12) line were easily detected and a total of 176 useable direct absorption scans were recorded, 65 for the S(10) and 111 for the S(12) line.

Twenty scans were taken as a function of laser current (convertible
to cm\textsuperscript{-1}) at each pressure of either the S(10) or S(12) line and coadded together. The twenty scans were first adjusted for drifts in laser temperature prior to coadding them. Only scans that had the same background curvature were coadded together. The coadded results were fitted using a polynomial least squares routine that excluded the region containing the absorption feature. Dividing the coadded results by these background fits yielded curves of transmission versus laser current. These curves were then coadded to obtain a final plot of transmission versus laser current at a given pressure. The S(10) line was characterized at pressures of 730, 734, and 837 Torr, while the S(12) line was observed at 729, 732, 837, 880, and 950 Torr. All data were taken for a path length of 5.016 km and a temperature of 297°K. The results were then compared to existing experimental data.
CHAPTER II
THEORETICAL DEVELOPMENT

II.1 Introduction

Many approaches have been used to accurately predict the positions, intensities, and shapes of absorption lines. The absorption line represents a transition by the molecule from a lower energy level to a higher energy level as a result of being exposed to electromagnetic radiation of the proper wavelength. The position (in cm$^{-1}$) of an absorption line, if multiplied by $\hbar c$, is simply the difference between the energies of the two levels involved in the transition. The energy eigenvalues for $N_2$ are obtained by solving Schrödinger's equation for a diatomic homonuclear molecule. A method for obtaining these eigenvalues is summarized in the next section. Discussions on the theory used to obtain line intensities and the derivative of the quadrupole moment are given in section II.3.

II.2 Diatomic Molecule Eigenfunctions and Eigenvalues

One of many approaches to the solution of the Schrödinger equation for a vibrating, rotating diatomic molecule is to methodically separate the electronic from the nuclear wavefunctions as was done by Born and Oppenheimer$^{14}$, and then to further separate the nuclear wave equations into an equation describing the translational motion of the center of mass of the molecule and one describing the internal motion. The internal
motion wave equation is then solved by separating the wavefunctions into a product of three wavefunctions; each a function of \( r, \theta, \) or \( \phi \) only. The following is a summary of the treatment by Pauling and Wilson\(^{15}\).

The mass of a nitrogen nucleus is several thousand times greater than that of an electron. This difference allows the electrons to complete many orbits about the nucleus before any change in the nuclear configuration can occur. Therefore, Born and Oppenheimer assumed that an approximate solution to the complete wave equation can be obtained by solving the wave equation for the electrons alone, with the nuclei in a fixed configuration, and then solving a wave equation for the nuclei alone assuming the electronic energy function is known. This complete wave function is:

\[
\sum_{j=1}^{r} \frac{1}{M_j} \nabla_j^2 \psi + \frac{1}{m_0} \sum_{i=1}^{s} \nabla_i^2 \psi + \frac{8\pi^2}{h^2} (W - V) \psi = 0 \tag{1}
\]

where \( M_j \) is the mass of the \( j \)-th nucleus, \( m_0 \) is the mass of each electron, \( r \) is the number of nuclei, and \( s \) is the number of electrons. The potential energy function, \( V \), is given by:

\[
V = \sum_{i,i'} \frac{e^2}{r_{ii'}} + \sum_{j,j'} \frac{Z_j Z_{j'} e^2}{r_{jj'}} - \sum_{i,j} \frac{Z_j e^2}{r_{ij}} \tag{2}
\]

If \( \xi \) represents the \( 3r \) coordinates of the \( r \) nuclei, \( x \) represents the \( 3s \) coordinates of the \( s \) electrons, \( n \) represents the electronic quantum numbers, and \( \nu \) represents the nuclear quantum numbers, then an approximate solution to (1) can be obtained of the following form:

\[
\psi_{n,\nu}(x, \xi) = \psi_n(x, \xi) \psi_{n,\nu}(\xi) \tag{3}
\]

where \( \psi_n(x, \xi) \) are electronic wave functions corresponding to different
sets of values of the electronic quantum numbers $n$ only, being independent of the nuclear quantum numbers $\nu$. At the same time, however, each of these functions is a function of $\xi$, the nuclear coordinates, as well as of $x$, the electronic coordinates. The functions $\psi_{n,\nu}(\xi)$ are nuclear wave functions which depend on the set of values of the electronic quantum numbers $n$ obtained for the electronic wave functions.

The electronic wave functions are obtained by solving a wave equation for the electrons alone, with the nuclei assumed to be stationary. This wave equation is:

$$\sum_{i=1}^{8} \psi_{n}(x,\xi) + \frac{8\pi^2 m}{\hbar^2} \{U_n(\xi) - V(x,\xi)\}\psi_n(x,\xi) = 0 \quad (4)$$

It is obtained from (1) by omitting the terms containing $V_j^2$, replacing $\psi$ with $\psi_n(x,\xi)$ and writing $U_n(\xi)$ in place of $W$. $V(x,\xi)$ is the complete potential function given in equation (2). Since $V$ depends on the values selected for the nuclear coordinates $\xi$, then $U_n$, the electronic energy values, and $\psi_n$ will also depend on $\xi$.

Equation (4) then is solved for all configurations of the nuclei. It has been shown that the values $U_n(\xi)$ are continuous functions of the nuclear coordinates $\xi$. In fact, for a free diatomic molecule, the electronic energy function (i.e., $U$) for the most stable electronic state ($n=0$) is a function only of the distance $r$ between the two nuclei and is a continuous function of $r$. A typical function $U(r)$ for a diatomic molecule is the Morse potential, which has these features and which will be discussed in more detail below in connection with the nuclear wave functions.
Having solved equation (4) for various nuclear configurations and obtaining $U_n(\xi)$, then $U_n(\xi)$ can be used as the potential function in the following nuclear wave equation:

$$
\sum_{j=1}^{r} \frac{1}{M_j} \nabla^2 \psi_{n,\mu}(\xi) + \frac{8\pi^2}{\hbar^2}(W_{n,\nu} - U_n(\xi))\psi_{n,\nu}(\xi) = 0
$$

(5)

where $W_{n,\nu}$ are the characteristic energy values for the entire molecule.

To summarize the Born-Oppenheimer approach, equations (4) and (5) are obtained by a procedure involving the expansion of the wave functions and other quantities in equation (1) as a power series in $(m_e/M)^4$, where $M$ is the average nuclear mass. This procedure is justified because the masses of the electrons are significantly less than the masses of the nuclei. This in turn allows the electrons to move with velocities much greater than that of the nuclei, and allows the electrons to complete many orbits about the nuclei before the nuclear configuration can change appreciably. Many of the cross terms in the power series expansion can then be neglected. Consequently the motion of the electrons can be quantized by solving equation (4), the electronic wave equation, for fixed nuclear configurations, and then use the electronic energy functions as potential energy functions in determining the motion of the nuclei from equation (5).

In studying transitions from rotational levels of the $\nu = 0$ vibrational level to rotational levels of the $\nu = 1$ vibrational level, no changes in the electronic configuration were involved. The wave equation of importance then is equation (5). The next step is to separate out the translational motion of the center of mass. This will leave a
wave equation for the internal motion of the molecule, from which the vibrational and rotational energy values can be derived.

If \( \Psi_{n, \nu} = \psi_{n, \nu}(x_1, y_1, z_1, x_2, y_2, z_2) \) and \( M_1 \) and \( M_2 \) are the masses of the two nuclei, and the Laplace operator is given by:

\[
\nabla^2 = \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2}, \quad i = 1, 2
\]

then the following transformations will separate the center of mass motion from the relative motion:

\[
x = \frac{M_1 x_1 + M_2 x_2}{M_1 + M_2}, \quad y = \frac{M_1 y_1 + M_2 y_2}{M_1 + M_2}, \quad z = \frac{M_1 z_1 + M_2 z_2}{M_1 + M_2}
\]

\[
rsin\theta\cos\phi = x_2 - x, \quad rsin\theta\sin\phi = y_2 - y, \quad r\cos\theta = z_2 - z
\]

where \((x, y, z)\) are the cartesian coordinates of the center of mass, and \((r, \theta, \phi)\) are the polar coordinates of the second nucleus relative to the first. With these substitutions, the usual definition of reduced mass \((\mu^{-1} = M_1^{-1} + M_2^{-1})\), and the wavefunction separation of

\[
\Psi_f(x, y, z, r, \theta, \phi) = F(x, y, z)\psi(r, \theta, \phi)
\]

the wavefunction for the internal motion of the molecule becomes:

\[
\left\{ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) \right\} + \frac{\hbar^2}{2\mu}(W - V)\psi = 0
\]

where \(W = W_T - W_{tr}\), i.e., the difference between the total energy eigenvalues and the translational energy eigenvalues.

Equation (10) can now be solved by assuming that \(V = V(r)\), and using the final separation of variables:

\[
\psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)
\]
The resulting eigenfunctions for $\theta$ and $\phi$ are:

$$\Phi(\phi) = e^{iM\phi}/\sqrt{2\pi}, \quad M = 0, \pm 1, \pm 2, \ldots \quad (12)$$

$$\Theta(\theta) = \sqrt{\frac{(2J + 1)}{2}} \frac{(J - |M|)!}{(J + |M|)!} \cos^{|M|}(\cos \theta) \quad (13)$$

There are two general methods\textsuperscript{17} of constructing potential curves from spectroscopic data and an expression for $U(r)$ is needed before a solution can be obtained for the radial wave functions. These wave functions, in turn, will allow the energy eigenvalues to be obtained. The first method is the graphical method of Rydberg which is designed to produce a curve which will give the observed vibrational and rotational energies, when these are computed using Bohr's theory with half-integral quantum numbers. The second method is to represent the potential curve with an analytical expression having a generally appropriate form and containing adjustable parameters. The curve most widely used is that of Morse\textsuperscript{16} while other useful curves are those of Rosen and Morse\textsuperscript{18}, Manning and Rosen\textsuperscript{19}, Pöschl and Teller\textsuperscript{20}, and Hylleraas\textsuperscript{21}. The Morse potential is given by

$$U(r) = D[1 - e^{-a(r - r_e)}]^2 \quad (14)$$

where $r_e$ is the equilibrium separation of the nuclei, and $D$ and $a$ are parameters which affect the depth or width of the potential curve, respectively.

The Morse potential is attractive at large distances, has a minimum of $-D$ at $r = r_e$ (the equilibrium separation), but produces a strong repulsion if the two nuclei approach even closer. The only portion where it does not fit the theoretically determined potential curves is at $r = 0$ where it should be infinity. The Morse function is, however, very large...
at \( r = 0 \) and its departure from infinity has little effect on the energy levels and wave function. Setting \( x = (r - r_e)/r_e \) and \( a = ar_e \), equation (14) can be rewritten as

\[
U(r) = D[1 - e^{-ax}]^2 = D(1 - 2e^{-ax} + e^{-2ax})
\]  
(15)

Around \( x = 0 \) (i.e., \( r = r_e \)), \( U(r) \) can expanded into a series

\[
U(r) = D(a^2x^2 - \ldots) = \frac{1}{2}M\omega^2(r - r_e)^2 - \ldots
\]  
(16)

with

\[
\omega^2 = \frac{2Da^2}{Mr_e^2}
\]  
(17)

For low-energy vibration terms the spectrum is not expected to deviate very much from that of a harmonic oscillator,

\[
E(v) = -D + \hbar \omega(v + \frac{1}{2}); \ v = 0,1,2,\ldots
\]  
(18)

where \( v \) is the vibrational quantum number. A more careful analysis yields the following eigenvalues

\[
E(v) = -D + \hbar \omega\{(v + \frac{1}{2}) - \frac{1}{Z}(v + \frac{1}{2})^2\}
\]  
(19)

where

\[
Z = \frac{2r_e}{\alpha \hbar} \sqrt{2MD}
\]  
(20)

The difference between equations (18) and (19) reflects the anharmonicity correction. The procedures to obtain either of these equations ignored the rotational energy of the molecule, which is much smaller than that of vibration. In order to derive an expression for the eigenvalues which includes the effects of both vibration and rotation, the Morse potential is used for \( U(r) \), i.e., equation (14), and the remaining wave equation in \( r \) is solved to obtain an expression for \( R(r) \) containing Associated Laguerre polynomials, i.e.,

\[
R(r) = (A/r) e^{-\frac{\alpha}{2}(2dy)^{b/2}} L^b_{\frac{1}{2}}(2dy)
\]  
(21)

where \( A \) is the normalization constant, and
Using equations (23-25), an expression for the term values (i.e., the eigenvalues, \( W_j \), divided by \( \hbar c \)) can be obtained. The result is:

\[
\frac{W_j}{\hbar c} = \omega_e (v+\frac{1}{2}) - \chi_e \omega_e (v+\frac{1}{2})^2 + J(J+1)B_e - D_e J^2 (J+1)^2 - \alpha_e (v+\frac{1}{2})J(J+1) \tag{26}
\]

where

\[
\omega_e = \frac{a}{2\pi c} \sqrt{\frac{2D}{\mu}} \tag{27}
\]

\[
\chi_e = \frac{\hbar \omega_e c}{4D} \tag{28}
\]

\[
B_e = \frac{\hbar}{8\pi^2 \mu \omega_e c} \tag{29}
\]

\[
D_e = \frac{\hbar^3}{128\pi^6 \mu^3 \omega_e^3 c^3 r_e^3} \tag{30}
\]

and

\[
\alpha_e = \frac{3\hbar^2 \omega_e}{16\pi^2 \mu^2 c^2 D} \left( \frac{1}{\ar_e} - \frac{1}{a^2 r_e^2} \right) \tag{31}
\]

The first two terms of equation (26) are exactly the same as those of equation (19), i.e., harmonic and anharmonic terms. The next three terms in equation (26) are: the rotational energy at a fixed distance \( r_e \), a negative term which takes into account the fact that larger rotational quantum numbers lead to an enlargement of the average distance independently of vibrations, and a coupling term of rotation and vibration.
which is negative because at higher vibrational quantum numbers the average nuclear distance increases beyond \( r_0 \) due to anharmonicity. The term values obtained for a vibrating rotator (or rotating oscillator) would be the sum of the vibrational energy of the anharmonic oscillator and the rotational energy of the nonrigid rotator but ignores the interaction (last term in equation (26)) of vibration and rotation.

Empirical and theoretical improvements have led to an expanded form of equation (26) for the vibrational-rotational term values, \( T(v,J) = \frac{W_{n\nu}}{\hbar c} \). This equation is given below:

\[
T(v,J) = \omega_v (v + \frac{1}{2}) - \omega_e x_v (v + \frac{1}{2})^2 - \omega_e y_v (v + \frac{1}{2})^3 - \omega_e z_v (v + \frac{1}{2})^4 + \omega_e x_e (v + \frac{1}{2})^5 - \\
\omega_e y_e (v + \frac{1}{2})^6 + ... + J(J+1)[B_{\omega} - \alpha_v (v + \frac{1}{2}) + \gamma_v (v + \frac{1}{2})^2 - \delta_v (v + \frac{1}{2})^3 \\
+ ...] - J^2(J+1)[D_{\omega} - \beta_v (v + \frac{1}{2}) + \pi_v (v + \frac{1}{2})^2 - ...] + J^3(J+1)[H_{\omega} \\
- \eta_v (v + \frac{1}{2}) + ...] - J^4(J+1)[L_{\omega}] + ...
\]  

(32)

In general, in an atom containing several electrons, the orbital angular momenta \( \ell_1, \ell_2, \ell_3, \ldots \) of the individual electrons are strongly coupled among themselves and the spins, \( s_1, s_2, s_3, \ldots \) can be considered to be strongly coupled among themselves. The orbital angular momenta vectorially add to form a resultant \( L \) and the spin angular momenta vectorially add to form a resultant \( S \), with the additional constraint that the resultant in each case be quantized. The energy levels of an atom are designated S, P, D, F, ... according to the value of \( L \); \( L=0 \) for S, \( L=1 \) for P, etc. The resultants \( L \) and \( S \) are then added together to give the total angular momentum \( J \) of the electrons of the atom. The total angular momentum can take on \( 2S+1 \) different values: \( L+S, L+S-1, L+S-2, \ldots, |L-S| \).

The atomic nuclei in a diatomic molecule are held together by the
electrons. The nuclei would otherwise repel one another due to the Coulomb force. Just as for individual atoms, the different electronic states of the molecule depend on the orbitals in which the electrons are. The electronic states for a molecule are designated $\Sigma, \Pi, \Delta, \ldots$ according to the value of $\Delta$ analogous to the $S, P, D, \ldots$ states of atoms. The angular momentum vector $\Delta$ is the component of the electronic orbital angular momentum along the internuclear axis of the diatomic molecule. For a given value of $L$, $\Delta$ can take on the values $\Delta = 0, 1, 2, \ldots, L$. The fact that the electronic states of a diatomic molecule are specified according to the component of $L$ rather than $L$ itself is $L$ is no longer a constant of the motion as it is for an individual atom. The motion of the electrons in an individual atom takes place in a spherically symmetric force field. Therefore $L$ is a constant of the motion as long as the effect of electron spin is small or neglected. In a diatomic molecule there is no longer a spherically symmetric force field, but there is symmetry about the axis connecting the two atoms. Therefore the component of the orbital angular momentum of the electrons about the internuclear axis is a constant of the motion. The total electronic angular momentum of a diatomic molecule about the internuclear axis is denoted $\Omega$, which is obtained by vectorially adding $\Delta$ and $\Sigma$. The molecular quantum number for spin, $\Sigma$, should not be confused with the symbol $\Sigma$ used to represent $\Delta = 0$. The quantum number $\Sigma$ can take on the values $S, S-1, S-2, \ldots, -S$.

Just as for individual atoms, if the resultant $S$ of the spin angular momenta of the molecule is zero, then the multiplicity $2S+1 = 1$ and the state is a singlet state while if $S$ is not zero then the states are referred to as multiplet states. An electronic energy level with $\Delta \neq 0$
splits into a multiplet of \(2S+1\) components. The energy levels for a molecule are written with the multiplicity as a superscript on the left side of the orbital angular momentum value, e.g., \(1\Sigma\) is a singlet state with a value of zero for the component of the orbital angular momentum along the internuclear axis.

The electronic energy levels, and the vibrational levels within each electronic level, of the \(N_2\) molecule are given in figure 2. The region around the vibrational levels \(v = 0\) and \(v = 1\) is shown in the enlarged view near the bottom of this figure. Figure 3 shows the rotational levels up to \(J' = 14\) within each of these vibrational levels and the absorptive transitions studied in this work, namely the \(S(8)\), \(S(10)\), and \(S(12)\) lines of \(N_2\). The \(N_2\) molecule was assumed to be in the electronic ground state, \(X^1\Sigma_g^+\), during all of the transitions that were studied herein. From the previous discussion it can be seen that \(\Lambda = 0\) from the use of the symbol \(\Sigma\), and the multiplicity is 1 (i.e., \(S = 0\)). The electronic ground state for any molecule is designated with an \(X\) preceding the value of \(\Lambda\). Excited states use \(A\), \(B\), \(C\), etc. in place of the \(X\). The subscript "g" from the German "gerade" indicates that \(N_2\) is even with respect to an inversion of the electronic wave function through the origin. That is, an even electronic wave function does not change as a result of this type of transformation. If it did change, the subscript would be a "u" from the German "ungerade" and the wave function would be odd. Electronic transitions are allowed only between even and odd levels (\(g \leftrightarrow u\), or \(u \leftrightarrow g\)) for homonuclear diatomic molecules. The superscript to the right of the value of \(\Lambda\) indicates the nuclear symmetry of the electronic wave function. This superscript is "+", as it is for \(N_2\), if upon an exchange of the two nuclei
Vibrational Levels \( v = 0 \) and \( v = 1 \) of the Electronic Ground State of \( N_2 \)

Figure 2. Energy Level Diagram of the \( N_2 \) Molecule
(from Herzberg\textsuperscript{25})
Figure 3. Rotational Levels of the 1←0 Vibrational Band of $N_2$ and Observed S-Branch Transitions
the electronic wave function of the molecule is left unchanged. In this case the electronic wave function is said to be symmetric in the nuclei. The superscript will be "-" if the electronic wave function is antisymmetric in the nuclei, i.e., if a factor of $-1$ is introduced into the electronic wave function upon an exchange of the two nuclei.

Thus far the resulting expression for the term values, i.e., equation (26), has expressions for the interaction of vibrational and electronic motions as well as the interaction of vibrational and rotational motions, but not the interaction of electronic and rotational motions. The interaction of vibrational and electronic motions was automatically included because the vibrational levels were chosen to fit the potential curve, equation (14), of the electronic state and because this potential curve represents the dependence of the electronic energy (including nuclear repulsion) on the internuclear distance. The interaction of vibrational and rotational motions was taken into account by considering the fact that, during vibration, the internuclear distance changes, which, in turn, changes the moment of inertia ($I_e = \mu r_e^2$) and consequently changes $B_e$, cf. equation (29). The paragraph following equation (31) identifies the term in equation (26) which is a result of the coupling between rotation and vibration.

As was mentioned earlier the total electronic angular momentum, $\Omega$, is obtained by vectorially adding $\Delta$ and $\Sigma$. The total angular momentum, $J$, of the molecule is obtained by adding $\Omega$ to $N$, the angular momentum of nuclear rotation. This procedure assumes a particular mode of coupling between $\Delta$, $\Sigma$, and $N$ to arrive at $J$, and this mode is known as Hund's case (a). The character of the energy spectrum of the molecule depends on the
kind of coupling between these three angular momenta, two which are
electronic and one which is rotational in nature. In Hund's case (a) the
energy of the coupling between the orbital (\(\Lambda\)) and spin (\(\Sigma\)) angular
momenta and the molecular axis is large compared to the distance between
the rotational levels. In other words, the interaction of the electronic
motions with the nuclear rotation is weak. In Hund's case (b), on the
other hand, the energy of the coupling between orbital and spin angular
momenta is small compared to the distances between the rotational levels.
The spin angular momentum, \(S\), is not coupled to the internuclear axis at
all, so it does not make sense to speak of \(\Sigma\); the projection of \(S\) onto
this axis. Consequently the vector \(\Omega\) is not defined. In case (b), \(\Lambda\) is
first added to \(N\) to form a resultant \(K\), then \(K\) is added to \(S\) (not \(\Sigma\)) to
obtain \(J\).

For the S-branch transitions studied in this work, the \(N_2\) molecules
were in the electronic ground state, which means \(\Lambda\) and \(S\) were both zero.
In this case the angular momentum of nuclear rotation, \(N\), was identical
to the total angular momentum, \(J\). Therefore, there was no need to modify
the term value expression for the interaction of electronic and rotational
motions (if the effects of nuclear spin are ignored).

The rotational levels of a diatomic molecule are classified according
to the behavior of the total eigenfunction with respect to reflection at
the origin. A rotational level is called positive or negative depending
on whether the total eigenfunction remains unchanged or changes sign for
such a reflection. This property described as positive or negative is
called 'parity'. As was discussed earlier, the complete eigenfunction of
a molecule, to a first approximation, is a product of an electronic, a
vibrational, and a rotational contribution. If $\Lambda = 0$, the electronic contribution will be unchanged by a reflection at the origin. The vibrational contribution always remains unchanged by a reflection at the origin because it depends only on the magnitude of the internuclear distance. The parity of the rotational levels, then, depends only on the rotational eigenfunction. So the rotational levels are positive or negative if $J$ is even or odd, respectively. A level is said to be symmetric (antisymmetric) if for an exchange of the nuclei, the total eigenfunction remains unchanged (or only changes its sign). For a homonuclear molecule, in a given electronic state, either the positive (even) rotational levels are symmetric and the negative (odd) are antisymmetric, or the positive are antisymmetric and the negative symmetric. If the nuclear spin is zero or neglected, there is a strict selection rule that prohibits transitions between symmetric and antisymmetric states. In the presence of nuclear spin, this selection rule is no longer absolute but, it is still very strict.

Every other line will be missing in the spectrum of a homonuclear molecule if the nuclear spin, $I = 0$, and the lines will alternate in intensity if $I \neq 0$. The different behavior of homonuclear molecules with and without nuclear spin is due to the fact that an exchange of nuclei when a nuclear spin is present does not necessarily lead to a completely identical state, since the nuclei may still differ by the orientation of their spins.

The nuclear spin vectors, $I$, of the two nuclei of a diatomic molecule form a resultant $T$, the total nuclear spin of the molecule. Since $I_1 = I_2 = I$ for a homonuclear diatomic molecule, the total nuclear spin will be
given by
\[ T = 2I, 2I-1, \ldots, 0 \]  \hspace{1cm} (33)
For \( N_2 \), \( I = 1 \) so \( T = 2, 1, 0 \). For symmetric levels only the even \( T \) values are possible, while for the antisymmetric levels only the odd values of \( T \) are possible. Referring to figure 3, the energy levels labelled with even \( J \) are symmetric, and those with odd \( J \) are antisymmetric. A state with a given \( T \) has a statistical weight \( 2T+1 \). For \( N_2 \), these statistical weights will be 5, 3, and 1. The statistical weights of the symmetric and antisymmetric rotational levels are obtained by adding separately the quantities \( 2T+1 \) for even and odd \( T \). The statistical weight of the symmetric levels for \( N_2 \) is found to be 6, while the statistical weight for the antisymmetric levels is 3. In general, the statistical weights, \( g_J \), for even \( T \) (symmetric for \( N_2 \)) and odd \( T \) (antisymmetric for \( N_2 \)) levels are given by \((2I+1)(I+1)\) and \((2I+1)I\), respectively. The ratio of these two numbers is
\[ R = \frac{I + 1}{I} \]  \hspace{1cm} (34)
For \( N_2 \) then, the even lines (transitions between even levels) in the spectrum will be twice as intense as the odd lines (transitions between odd levels). As will be discussed later, the tuning range of the diode laser included the S(9) and S(11) lines, but these lines are half as intense as the S(8), S(10), or S(12) lines for which the signal-to-noise ratio was already very small. Therefore no attempt was made to detect these odd lines.

If the interaction with an electromagnetic field (laser) is introduced into the Schrödinger equation of a diatomic system, it is found that a non-zero probability arises of finding the system in an energy state \( E_n \)
if it were originally in an energy state $E_n$ provided the spectral range of the laser radiation contains the wavenumber $\nu$ such that $\nu = (E_n - E_n)/hc$. In other words a photon is absorbed by a diatomic molecule only when the energy of the photon is equal to the difference in energies between two possible energy eigenstates. For electronic transitions, the two eigenstates correspond to two orbits, and the absorbed energy forces an electron to jump from the orbit of lower energy to the orbit of higher energy. For vibration-rotation transitions, in which small rotational excitations are superimposed onto the nuclear vibrational motion of a molecule, the diatomic molecule will change to a different vibrational/rotational pattern upon absorbing a photon of the proper energy.

The probabilities of the transitions are computed using the eigenfunctions of the two states that are involved. The interaction of an electromagnetic wave with the electric quadrupole moment of $N_2$ will be described within the expression for the transition probability by the matrix element or integral of the product of the initial (complex conjugate of) and final diatomic molecule eigenfunctions with the usual expression for the quadrupole moment operator placed in between. If the matrix element is non-zero then a transition can occur between the eigenstates. If it is zero, as it would be for $N_2$ for electric dipole transitions, then the transition is forbidden.

These probabilities will be linearly dependent on time. Dividing through by time, the transition probability per unit time is obtained for a given photon energy (wavenumber). The transition rate for a single photon with a wave vector $|k| = \omega/c$ cannot be measured in practice. In fact with any laser source $k$ will range from $k$ to $k + \Delta k$. The transition
rate will be the transition probability per unit time summed over the range of \( k \) values. The transition rate will then contain a function which quantifies the density of states (energies) in this wave vector interval. Multiplying the transition rate by the photon energy \((\hbar \omega)\) converts it into an intensity.

The computation of the matrix element gives rise to selection rules, i.e., conditions that must be met in order for the transition to be possible (or equivalently in order for the matrix element to be non-zero). For electronic transitions the selection rule for the total angular momentum \( J \)

\[
\Delta J = 0, \pm 1 \quad \text{with} \quad J = 0 \rightarrow J = 0
\]

always holds (assuming dipole radiation). Furthermore, the symmetry selection rules hold quite generally. Positive terms combine only with negative, and vice versa:

\[
+ \leftrightarrow -, \quad + \rightarrow +, \quad - \rightarrow -
\]

and for identical nuclei, symmetric terms combine only with symmetric and antisymmetric only with antisymmetric, or

\[
s \leftrightarrow s, \quad a \leftrightarrow a, \quad s \rightarrow a
\]

Finally, in the case of nuclei with equal charge (and as mentioned earlier) the selection rule is that even electronic states combine only with odd, that is

\[
g \leftrightarrow u, \quad g \rightarrow g, \quad u \rightarrow u
\]

For example, \( \Sigma_g \leftrightarrow \Sigma_u \), but \( \Sigma_g \rightarrow \Sigma_g \). For homonuclear diatomic molecules such as \( \text{N}_2 \), this selection rule follows immediately from (36) and (37) because for identical nuclei all the positive levels are symmetric and the negative antisymmetric in an even electronic state and vice versa for
an odd state. Equation (38) holds for heteronuclear molecules as well, even if the symmetric-antisymmetric property is not defined, and is independent of whether \( \Delta \) is defined or not. Equation (38) does not hold quite rigorously if the influence of rotation is taken into account in the cases where the symmetric-antisymmetric property is not defined.

Moving as a specific example to \( ^1\Sigma - ^1\Sigma \) transitions, \( \Delta K = 0 \) is forbidden, or since \( J = K \), \( \Delta J = 0 \) is forbidden. So only transitions with \( \Delta J = \Delta K = \pm 1 \) are possible which gives rise to a single \( P \) and a single \( R \) branch. Summarizing the above selection rules, the possible electronic transitions include \( ^1\Sigma^+ - ^3\Sigma^+ \), \( ^3\Sigma^+ - ^1\Sigma^+ \), \( ^1\Sigma^- - ^3\Sigma^- \), and \( ^3\Sigma^- - ^1\Sigma^- \).

For a harmonic oscillator, the selection rule for transitions between vibrational levels is \( \Delta \nu = \pm 1 \), but for the anharmonic oscillator, overtones (i.e., \( \Delta \nu = 2, 3, ... \)) can also occur. However the transition probability decreases rapidly with increasing \( \Delta \nu \).

For dipole transitions the selection rules for diatomic molecules are \( \Delta \Delta = \pm 1 \), \( \Delta \nu = \pm 1 \), and \( \Delta J = 0, \pm 1 \).

As was already discussed, transitions between symmetric (+) and antisymmetric (-) rotational states of a homonuclear diatomic molecule are forbidden unless the nuclear spin differs from zero. Transitions can occur between symmetric \(+ \leftrightarrow +\) or between antisymmetric levels \(- \leftrightarrow -\). Since the nuclear spin is equal to one for \( N_2 \), then this rule is not strict but is valid most of the time.

Rotation-vibration spectra of homonuclear diatomic molecules are rigorously forbidden as ordinary dipole radiation (since homonuclear diatomic molecules do not have a permanent dipole moment) but may occur as quadrupole radiation. Transitions with \( \Delta J = 0, \pm 2 \) (Q, S, and O branches)
are possible between two vibrational levels of a given $\Sigma_g$ or $\Sigma_u$ state. However, there cannot be a transition from a $J = 0$ level in the initial to the $J = 0$ level in the final state.

If the ground state of $N_2$ were a $\Pi$ rather than $\Sigma$ electronic state, there would be the possibility of dipole radiation as well as $\Lambda$-doubling. Two transitions would not necessarily be observed, i.e., a splitting of each line in electronic transitions as a result of $\Lambda$-doubling. The splitting or doubling refers to the fact that each energy level is split into two ($a + \Lambda$ and $a - \Lambda$ level) and these two are close together. One of these two levels will be $+$ while the other will be $-$. Transitions will be governed by the selection rule $+ \leftrightarrow -$. A splitting of each line will occur for $^1\Pi - ^1\Pi$ transitions, but not for $^1\Pi - ^1\Sigma$ transitions.

To get an idea of the difficulty involved in measuring a quadrupole absorption line, previous calculations on $H_2$ and HCl yielded a ratio of integrated absorption coefficients for these two gases (quadrupole vs. dipole) of $8.1 \times 10^{-9}$, i.e., the $H_2$ quadrupole lines were nine orders of magnitude smaller than a HCl dipole line.

### II.3 Quadrupole Line Intensity

The mechanisms\textsuperscript{28} responsible for the attenuation of an electromagnetic disturbance as it propagates through a medium are classified into two categories: absorption and scattering. Consider a beam of collimated, monochromatic radiation of irradiance $I_\lambda$ which is incident upon an elemental volume $dv$ of an attenuating medium. It is reasonable to assume that the fraction of the radiation attenuated in passing through a thin
layer dx of the medium is proportional to the thickness, i.e.,

\[ \frac{I(x) - I(x + dx)}{I(x)} = \frac{dI(\lambda)}{I(\lambda)} = -k(\lambda)dx \]  

(39)

where \( k(\lambda) \), the extinction coefficient, is the constant of proportionality, depending on the nature of the medium contained in the elemental volume \( dv \) as well as on the wavelength of the radiation. Assuming that the attenuation results from absorption and scattering and that these mechanisms act independently, then equation (39) becomes

\[ \frac{dI(\lambda)}{I(\lambda)} = -(a + \beta)dx \]  

(40)

where \( a \) is the absorption coefficient, and \( \beta \) is the scattering coefficient.

Both \( a \) and \( \beta \) are functions of the wavelength of the radiation.

Under suitable conditions, the absorption of each absorbing element is independent of the concentration of that element. Thus the absorption coefficient is proportional to the number of absorbing elements encountered per unit path length and hence is proportional to the concentration \( n_a \) of those elements, or

\[ a = \sigma_{abs}n_a \]  

(41)

where \( \sigma_{abs} \) (usually a function of wavelength) is the absorption coefficient per unit of concentration. Equation (41) is known as Beer's law.

The previous assumption concerning the independence of \( \sigma_{abs} \) and \( n_a \) may be invalid in some cases. Changes in concentration, for example, may alter the nature of the absorbing molecules or may cause interactions between them. The conditions under which the \( N_2 \) data were taken were such to satisfy Beer's law. The concentration (pressure) within the White cell
was controlled and not excessive, and reasonably pure \( \text{N}_2 \) was used, minimizing any interactions.

In the same manner the scattering coefficient \( \beta \) may be written as
\[
\beta = \sigma_{\text{sca}} n_s
\]
where \( n_s \) is the concentration of the scattering elements, and \( \sigma_{\text{sca}} \) is the scattering coefficient per unit of concentration.

Since \( \sigma_{\text{abs}} \) and \( \sigma_{\text{sca}} \) have the dimensions of area, they are referred to as absorption and scattering cross sections. Using equations (41) and (42) in equation (40) yields
\[
\frac{dI(\lambda)}{I(\lambda)} = - (\sigma_{\text{abs}} n_a + \sigma_{\text{sca}} n_s) dx
\]
which integrates to
\[
I(\lambda) = I_0(\lambda) \exp[-(\sigma_{\text{abs}} n_a + \sigma_{\text{sca}} n_s) x]
\]
where \( I(\lambda) \) is the transmitted spectral irradiance and \( I_0(\lambda) \) is the spectral irradiance at the front surface of the medium being considered. Equation (44) is known as the Beer-Lambert Law.

The total extinction is the sum of absorption and scattering terms. The scattering in this case is the usual Rayleigh scattering as well as rotational and vibrational Raman scattering, i.e.,
\[
\sigma(\lambda) = \sigma_{\text{abs}}(\lambda) + \sigma_{\text{Rayleigh}}(\lambda) + \sigma_{\text{Raman rot.}}(\lambda) + \sigma_{\text{Raman vib.}}(\lambda)
\]
Rayleigh scattering arises when the incident radiation (a time-varying electric field) induces a varying dipole moment in the molecules that are in the path of the laser beam. This varying dipole moment gives rise to radiation of the same frequency as the incident beam, and this radiation can go in any direction. The net effect is that this scattering removes
photons from the laser beam. Rayleigh scattering is essentially elastic. Only the very small amount of energy necessary to conserve momentum between the photon and the scattering molecule is exchanged (Doppler-Brillouin effect). Unlike Raman scattering, the wavelength of the Rayleigh-scattered photon is essentially unchanged.

If the incident light is scattered inelastically, the process is called the Raman effect, i.e., the incident photon gives up part of its energy to the scattering system or takes energy from it. The amount given up or taken away has to equal the difference between the energies, $\Delta E$, of the stationary states of the molecule. The scattered photon will have an energy equal to that of the original photon $\pm \Delta E$. The Raman lines which are displaced toward longer wavelengths are called Stokes lines, and those toward shorter wavelengths are called anti-Stokes lines. As mentioned earlier there are two types of Raman scattering, i.e., vibration-rotation scattering (or simply vibrational scattering) and pure rotational scattering. The Raman vibrational scattering shift, $\Delta E$, for $N_2$ is 2331 cm$^{-1}$ (if wavenumber units are used).

The S(10) and S(12) lines of $N_2$ are at 2418.6526 cm$^{-1}$ and 2433.5894 cm$^{-1}$, respectively, which correspond nominally to the wavenumbers selected for the incident laser beam photons. In this experiment, the InSb detectors had a spectral range of sensitivity from 2000 cm$^{-1}$ to 3333 cm$^{-1}$. Therefore, the detectors could not detect the scattered light due to Raman vibrational scattering, but the number of photons removed from the beam can be simply calculated given the appropriate Raman vibrational scattering cross section.
Pure rotational Raman scattering will produce photons with wavenumbers within the sensitivity range of the InSb detectors. These lines are, to a first approximation, spaced equally far apart (i.e., by 4B where B = 1.989574 cm\(^{-1}\) for \(N_2\)), except for the spacing between the incident energy and the first line (which is 6B).

Even though Rayleigh and pure rotational Raman scattered light could be detected by an InSb detector, this light would have had to pass through a small (less than one-inch-square) field stop within a small range of angles prior to exiting the White cell to be detected. Since this scattering is isotropic, i.e., in all directions, it can be assumed that all scattered photons were removed from the beam and not detected.

The Rayleigh backscattering differential cross section\(^{32}\) of \(N_2\) at 694.3 nm is \(2.14 \times 10^{-28} \text{ cm}^2/\text{sr}\). Assuming isotropic scattering this differential cross section, \(d\sigma/d\Omega\), can be converted to a total cross section, \(\sigma\), by multiplying by \(4\pi\) to get \(2.69 \times 10^{-27} \text{ cm}^2/\text{molecule}\). All of these scattering cross sections are a function of \(\lambda^{-4}\) where \(\lambda\) is wavelength. Scattering is greater at shorter wavelengths. To correct this cross section for the wavelength used to characterize the \(S(10)\) line of \(N_2\), the cross section is multiplied by

\[
\frac{(0.6943 \mu\text{m})^4}{(4.1345 \mu\text{m})^4} = 7.95 \times 10^{-4}
\]

So the Rayleigh cross section, \(\sigma_{\text{Rayleigh}}\), is \(2.14 \times 10^{-38} \text{ cm}^2/\text{molecule}\) at 4.1345 \(\mu\text{m}\).

The Raman vibrational scattering cross section\(^{31}\) at 488.0 nm is \(7.03 \times 10^{-38} \text{ cm}^2/\text{molecule}\). The wavelength correction in this case will be

\[
\frac{(0.4880 \mu\text{m})^4}{(4.1345 \mu\text{m})^4} = 1.94 \times 10^{-4}
\]
The Raman vibrational scattering cross section, $\sigma_{\text{Raman vib.}}$, is then $1.36 \times 10^{-33}$ cm$^2$/molecule at 4.1345 µm.

Raman rotational scattering is usually an order of magnitude stronger than vibrational scattering$^{33}$. The Raman rotational cross section, i.e., $\sigma_{\text{Raman rot.}}$, is approximately $1.36 \times 10^{-32}$ cm$^2$/molecule.

The number of molecules per unit volume, $n$, can be determined from the ideal gas law

$$pV = NkT, \text{ or } n = N/V = p/kT$$  (48)

The pressures ranged from 730 Torr to 950 Torr, and $T = 297^\circ$K. Using the ideal gas law with $p = 730$ Torr, $n$ is found to be $2.37 \times 10^{19}$ molecules/cm$^3$. The path length $x = 5.016 \times 10^5$ cm, giving $1.19 \times 10^{26}$ molecules/cm$^2$ for $nx$. The factors $\exp[-n\sigma_{\text{Rayleigh}}x]$, $\exp[-n\sigma_{\text{Raman vib.}}x]$, and $\exp[-n\sigma_{\text{Raman rot.}}x]$ are then approximately $1.0 - 2.55 \times 10^{-6}$, $1.0 - 1.62 \times 10^{-8}$, and $1.0 - 1.62 \times 10^{-7}$, respectively, which, when multiplied together give $1.0 - 2.56 \times 10^{-6}$. Under these conditions, the Beer-Lambert equation becomes

$$I = I_o \left[\exp(-n\sigma_{\text{abs}}x)\right](1.0 - 2.56 \times 10^{-6})$$  (49)

Since the transmission $\tau = I/I_o$ is what has been measured, the factor $\exp(-n\sigma_{\text{abs}}x)$ which is totally due to absorption by $N_2$ can be obtained from:

$$(I/I_o)(1.0000256) = \exp(-n\sigma_{\text{abs}}x)$$  (50)

For narrow line widths such as for $N_2$, the extinction (transmission) at the line center can be corrected for scattering losses to determine that due to absorption alone. The total extinction was measured to be on the order of 1% for the $S(10)$ or $S(12)$ lines of $N_2$. An extinction of 1% corresponds to a transmission of 0.99 before correction, 0.99003 after
correction. The absorption would be quoted as 0.997\% rather than 1.000\% at line center.

The correction factors for the S(10) and S(12) line centers as a function of the pressures under which the data were taken are given in Table 1.

**TABLE 1. SCATTERING LOSS CORRECTION FACTORS**

<table>
<thead>
<tr>
<th>Pressure(T)</th>
<th>Factor</th>
<th>Pressure(T)</th>
<th>Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>730</td>
<td>1.0000256</td>
<td>729</td>
<td>1.0000262</td>
</tr>
<tr>
<td>734</td>
<td>1.0000258</td>
<td>732</td>
<td>1.0000264</td>
</tr>
<tr>
<td>837</td>
<td>1.0000294</td>
<td>837</td>
<td>1.0000301</td>
</tr>
<tr>
<td></td>
<td></td>
<td>880</td>
<td>1.0000317</td>
</tr>
<tr>
<td></td>
<td></td>
<td>950</td>
<td>1.0000342</td>
</tr>
</tbody>
</table>

As can be seen from this table, the amount of scattering increases both with pressure (number of molecules) and increases as the wavelength decreases ($\lambda^{-4}$ dependence).

The scattering losses are small in this case, and for shorter path lengths and/or lower pressures losses due to scattering can usually be neglected. In order to show the relationships between the transition probability, absorption coefficient, and line intensity, the Beer-Lambert equation in the absence of scattering losses would be

$$I(\nu) = I_o(\nu)\exp[-k_{\text{abs}}(\nu)nx]$$

(51)

where $I_o(\nu)$ is the intensity of the source of radiation in the absence of the gas under study, $I(\nu)$ is the intensity of the radiation at wavenumber $\nu$ after passing through the gas, $k_{\text{abs}}(\nu)$ is the absorption coefficient, $n$ is the concentration, and $x$ is the optical path length.

For an optically thin sample, the amount of light absorbed by a gas in going from state m to state n will be
where the incident intensity $I_o(\nu)$ is assumed to be constant over the width of the line. If $\rho_{mn}$ is the density of radiation in the incident beam of wavenumber $\nu_{mn}$, then the energy absorbed from the incident beam of 1 cm$^2$ cross section per second will be given by

$$I_{abs}^{nm} = \int [I_o(\nu) - I(\nu)]d\nu = I_o(\nu) \rho_{mn} B_{mn} \chi h c \nu_{mn}$$  \hspace{1cm} (52)$$

where $n_m$ is the number of molecules/cm$^3$ in the lower state $m$ and $B_{mn}$ is the Einstein transition probability of absorption. The factor $\rho_{mn} B_{mn}$ represents the number of transitions per cm$^3$ per second produced by the incident radiation. If $I_{abs}^{nm} = c \rho_{mn}$ is the intensity of the incident radiation (i.e., energy falling on 1 cm$^2$ per second) then

$$I_{abs}^{nm} = \rho_{mn} n_m B_{mn} \chi h c \nu_{mn}$$  \hspace{1cm} (53)$$

Substituting equation (52) into (54) and taking $I_{abs}^{nm} = I_o(\nu)$, the integral of the absorption coefficient, $S$, or simply the integrated absorption becomes

$$S = \int k_{abs}(\nu)d\nu = B_{mn} \chi h c \nu_{mn}$$  \hspace{1cm} (55)$$

It can be shown for dipole transitions that

$$B_{mn} = \frac{8\pi^3}{3hc} |R_{mn}|^2$$  \hspace{1cm} (56)$$

where $R_{mn}$ is the matrix element of the transition. In the case of $N_2$ the operator used in computing the matrix element will be that of the electric quadrupole moment. Substituting equation (56) into (55) yields

$$S = \int k_{abs}(\nu)d\nu = \frac{8\pi^3}{3hc} \nu_{mn} |R_{mn}|^2$$  \hspace{1cm} (57)$$

It would appear to be a straightforward procedure to get the integrated absorption from the measured data by rearranging equation (51) and substituting into equation (55):
In practice, however, this equation is not applicable to the observed spectrum. Equation (58) is valid only for a spectrometer with infinite resolving power. In an actual laboratory spectrometer, the spectrum is always distorted by the finite resolving power of the instrument. It has been shown that under certain conditions, the measured value of $S$ using equation (58) approaches the true value, i.e., the value measured with a distortion free spectrometer, in the limit as $n_{x}$ goes to zero\textsuperscript{35}.

A technique commonly used when it is possible to isolate individual spectral lines is the "curve-of-growth" method. Using this method it is possible to derive both the strength and width of individual lines from a measurement of the equivalent width under varying conditions. The equivalent width is defined as

$$W = \int [1 - \exp(-k_{abs}(\nu)n_{x})]d\nu$$  \hspace{1cm} (59)

Using equation (51), the equivalent width can be written as

$$W = \int [1 - I(\nu)/I_{o}]d\nu = (1/I_{o}) \int [I_{o} - I(\nu)]d\nu$$  \hspace{1cm} (60)

for constant $I_{o}$. If $I_{o}$ is not constant, then $1/I_{o}$ is replaced in equation (60) by $1/(I_{o})$ where $\langle I_{o} \rangle$ is the average value of $I_{o}$ over the interval of integration. The integral in equation (60) is simply the area between the spectral line and the 100% transmission line. The term equivalent width is used because $W$ is the width in cm\textsuperscript{-1} of a rectangle of height $I_{o}$ that has the same area as that between the spectral line and the 100% transmission line. The equivalent width is independent of the resolving power of the spectrometer if, over the width of the response function of the spectrometer, either $I_{o}$ varies linearly with $\nu$ and the response function is sym-
metric or $I_o$ is constant.\(^{35}\)

The absorption coefficient can always be written in the form
\[ k_{\text{abs}}(\nu) = S \, f(\nu - \nu_o) \]  (61)
where $S$ is a constant independent of line shape and where the function $f(\nu - \nu_o)$ is a Doppler, Voigt, or Lorentz shape function which is normalized such that
\[ \int f(\nu - \nu_o) = 1 \]  (62)

For pressures in the range of 0.1 to 1 Torr, the line shape is known to be Gaussian and the line width is equal to the Doppler width. Neglecting collisional narrowing, if the pressure is in the range of several hundred Torr, the line shape is Lorentzian. At intermediate pressures the Voigt profile must be assumed.\(^{38}\) The pressures used in this study were greater than or equal to 730 Torr indicating that the line shape should be Lorentzian.

The Lorentz or collision-broadened profile is given by
\[ f(\nu - \nu_o) = (b_L/\pi)/[(\nu - \nu_o)^2 + b_L^2] \]  (63)
where $b_L$ is the Lorentz or collision-broadened half-width. It is defined as one-half the full-width of the line measured at the points where $k_{\text{abs}}(\nu) = \frac{1}{2} k_{\text{abs}}(\nu_o)$, $\nu_o$ being the wavenumber corresponding to the line center or minimum transmission. The half-width is generally linearly dependent on the gas pressure. For a pure gas sample
\[ b_L = b_L^o \, p \]  (64)
For a mixture of gases
\[ b_L = \Sigma b_i^o \, p_i \]  (65)
where $b_i^o$ is the half-width of the line broadened by gas $i$ at some standard pressure and $p_i$ is the partial pressure of that gas. Both constants $b_L^o$
and $b^L$ are called Lorentz broadening coefficients.

The equivalent width can be written as a function of $S$, $n_x$, and $b_L$:

$$W = 2\pi b_L e^{-u} [I_0(u) + I_1(u)]$$  \hspace{1cm} (66)

where $u = S n_x / 2 \pi b_L$ and $I_0(u)$, $I_1(u)$ are modified Bessel functions of the first kind with imaginary arguments. An iterative method is used to find $S$ from $W$ by using a starting value for $S$ taken from previous measurements or theoretical calculations. It can be shown that if $u \rightarrow 0$, then $W \rightarrow S n_x$. This is the so-called weak-line limit or linear region of the curve-of-growth.

In a typical experiment to determine Lorentz broadening coefficients, a number of spectra are recorded at different pressures. The half-width at half-maximum values obtained in each spectrum can be plotted as a function of pressure to fit a straight line whose slope corresponds to $b^L$ in equation (64).

The value of $S$ can also be determined directly from the value of the minimum transmittance $\tau(\nu_0)$ provided the line shape is known. This is usually possible if the width of the instrument line shape function is negligible in comparison to the line width of the line being measured. For a Lorentz line at $\nu = \nu_0$:

$$[f(\nu - \nu_0)]_{\nu = \nu_0} = 1/(\pi b_L)$$  \hspace{1cm} (67)

Inserting this into equation (61) and noting that the gas concentration, $n$, can be expressed in terms of the pressure $p$ from equation (48) (The additional factor of $k T$ is combined with $k_{\text{abs}}$, changing the units on $k_{\text{abs}}$ from concentration$^{-1}$distance$^{-1}$ to pressure$^{-1}$distance$^{-1}$), the transmission at line center can be written as

$$\tau(\nu_0) = \exp(-k_{\text{abs}} p x) = \exp(-p x S / \pi b_L)$$  \hspace{1cm} (68)
which leads to

\[ S = (\pi b_p/p_x) \ln[1/\tau(\nu_o)] \tag{69} \]

For a pure gas sample equation (64) can be substituted into equation (68) to obtain

\[ \tau(\nu_o) = \exp[-Sx/\pi b_p^2] \tag{70} \]

which shows that \( \tau(\nu_o) \) is independent of pressure. In the case of a Lorentz line for a pure gas, \( \tau(\nu_o) \) remains fixed as the pressure is increased provided the path length, \( x \), is not changed\(^{37} \).

The integrated absorption of a quadrupole line \( \nu',J' \rightarrow \nu,J \) is theoretically given\(^{39} \) by:

\[ S_{\nu}(T) = \frac{8\pi^5}{15 \ h c} \nu^3 e^{-E/kT} g_j \frac{(2J + 1)}{Z(T)} |<J 0 2 0|J' 0>|^2 |<\nu|Q|\nu'>|^2 \tag{71} \]

where \( \nu \) is the frequency of the transition given in wavenumber units (cm\(^{-1}\)), \( Z(T) \) is the rotational partition function, \( g_j \) is the nuclear spin statistical weight (not to be confused with the Landé g-factor), and \( <j_1 m_1 j_2 m_2 |jm> \) is a Clebsch-Gordan coefficient, which is computed from the following expressions:

\[ \frac{3J(J-1)}{2(2J - 1)(2J + 1)} \] for 0 lines \( (J' = J - 2) \) \hfill (72a)

\[ \frac{J(J + 1)}{(2J - 1)(2J + 3)} \] for Q lines \( (J' = J) \) \hfill (72b)

\[ \frac{3(J + 1)(J + 2)}{2(2J + 1)(2J + 3)} \] for S lines \( (J' = J + 2) \) \hfill (72c)

Only S lines were observed in this work, specifically the S(8), S(10), and S(12) lines of \( N_2 \). The square of the Clebsch-Gordan coefficients for \( J = 8, 10, \) and 12 are then 270/646 (\( \approx 0.418 \)), 396/966 (\( \approx 0.410 \)), and 546/1350 (\( \approx 0.404 \)), respectively. The nuclear spin statistical weight, \( g_j \),
will be equal to 6 because all of the \( J \) values are even. A discussion of \( g_j \) was given following equation (33).

The rotational partition function \( Z(T) \) is given\(^4\) by:

\[
Z(T) \sim \sigma^{-1} g^2 \beta/\beta^3 \left[ 1 + \frac{\beta^2}{90} + \frac{8\beta^3}{2835} + \ldots + \kappa g^{-1} \pi^{3/2} e^{-\beta/12 \pi^2/4 \beta^{-1/2}} \right] f_c \tag{73}
\]

where \( \beta = \hbar c B / k T \)
\( B = 1.989574 \pm 0.000012 \text{ cm}^{-1} \) (from Bendtsen\(^8\))
\( g = \) nuclear spin multiplicity = \( 2I + 1 = 3 \)
\( \sigma = \) symmetry number = 2
\( f_c = \) centrifugal distortion correction to the rigid-rotator partition function = \( 1 + 2D/B\beta \)
\( D = (5.76 \pm 0.03) \times 10^{-8} \text{ cm}^{-1} \) (from Bendtsen\(^8\))
\( \kappa = \pm 1 \) according to whether the resultant statistics are Bose or Fermi. For \( N_2 \), \( \kappa = + 1 \)

Using these expressions, \( Z(297^o K) = 468.67 \).

Pettitt and Danchura\(^41\) gave a value of 27.1135 for the rotational partition function of \( N_2 \) at 77\(^o\)K, which was computed from \( Z(T) = 1/\beta \).

Even though they note that they have ignored spin statistics, they have in fact also ignored the correction for centrifugal distortion, and the symmetry factor (i.e., number of different but distinguishable spatial orientations). The correct value for \( Z(T) \) at 77\(^o\)K using equation (73) is 122.5734, which is a factor of 4.5 larger than that used by Pettitt and Danchura.

Given the observed integrated absorption, equation (71) can be solved for the quadrupole moment matrix element. The matrix element can in turn be approximated by a simple expression involving the first derivative of the quadrupole moment and various molecular constants.

Expanding the quadrupole moment in a Taylor series expansion about the equilibrium separation distance, \( r_e \):
Using the harmonic oscillator approximation, so that the harmonic oscillator wave functions, \( u_n(x) \), can be used, the matrix element can be written (keeping only the first two terms of equation (74)):

\[
Q = Q_e + \left( \frac{\partial Q}{\partial r} \right) r_e (r - r_e) + \ldots
\]  

(74)

The factor \( Q_e \) in the first integral is a constant, namely the quadrupole moment when \( r = r_e \). Therefore \( Q_e \) can be pulled outside the integral. As shown in Schiff\(^4\) the first integral is zero when \( n \neq m \), a result of the normalization process. In the second integral, the first derivative of \( Q_e \), evaluated at \( r_e \), is also a constant and can be removed from the integral. The remaining operator, \( (r - r_e) \), can be written as \( x \), and from Schiff:

\[
\frac{(1/\alpha)[(n+1)/2]^{1/2}, m = n + 1}{\int u_n^*(x) x u_n(x) \, dx = (1/\alpha)(n/2)^{1/2}, m = n - 1}
\]

(76)

\[
0, \quad m = n
\]

In this case \( n = \nu \), and \( m = \nu + 1 \), and \( \alpha^2 \) is given by \( \mu \omega/\hbar \). Equation (75) can then be written

\[
\langle \nu | Q | \nu + 1 \rangle = \left( \frac{\partial Q}{\partial r} \right) r_e \left( \frac{\hbar}{2\mu \omega} \right)^{1/2} \sqrt{\nu + 1}
\]

(77)

The middle factor in this equation, \( (\hbar/2\mu \omega)^{1/2} \), can be rewritten in terms of the molecular constants, \( B_e \), \( r_e \), and \( \omega_e \):

\[
\left( \frac{\hbar}{2\mu \omega} \right)^{1/2} = \left( \frac{\hbar}{4\pi \mu a \omega r_e} \right)^{1/2} = \left( \frac{\hbar}{4\pi \mu a \omega r_e} \right)^{1/2} = \left( \frac{\hbar}{4\pi \mu \omega} \left( \frac{2\alpha^2 \mu}{2\omega^2 r_e^2 \mu} \right) \right)^{1/2}
\]

(78)

\[
= \left( \frac{\hbar}{4\pi \mu \omega} \left( \frac{\mu}{2\omega^2 \mu r_e^2 / 2\alpha^2} \right) \right)^{1/2} = \left( \frac{\hbar}{4\pi \mu \omega / 2a} \right)^{1/2} = \frac{1}{r_e} \left( \frac{\hbar}{4\pi \mu \omega / 2a} \right)^{1/2}
\]

(79)
= \left( \frac{h}{8\pi^2\mu r_e^2c} \frac{\mu}{2D} \frac{2\pi c}{a} \right)^{\frac{1}{2}} = r_e \left[ \frac{(h/8\pi^2\mu r_e^2c)}{(a/2\pi c)(2D/\mu)^{\frac{1}{2}}} \right]^{\frac{1}{2}} \quad (80)

The substitution of \( a \) for \( ar_e \) in equation (78) was taken from the sentence introducing equation (15), and the substitution for \( D \) in equation (79) was taken from equation (17) with \( \mu \) in place of \( M \). The last expression in equation (80) can be simplified using equations (27) and (29) to give \( r_e(B_e/\omega_e)^{\frac{1}{2}} \). Inserting this result into equation (77) gives

\[ <\nu|0|\nu+1> = \left( \frac{3Q}{4r} \right) r_e \omega_e \left( \frac{B_e}{\omega_e} \right)^{\frac{1}{2}} \sqrt{\nu + 1} \quad (81)\]

where \( \nu = 0 \), \( r_e = 1.097700 \ \text{Å} \), \( B_e = 1.989574 \ \text{cm}^{-1} \), and \( \omega_e = 2358.57 \ \text{cm}^{-1} \). The constants \( r_e \) and \( B_e \) were taken from Bendtsen\(^8\), and \( \omega_e \) was taken from Huber and Herzberg\(^43\). Upon substitution of this expression for the matrix element into equation (71), the observed data can be used to obtain values for the derivative of the quadrupole moment evaluated at \( r_e \), the equilibrium separation distance.
CHAPTER III

EXPERIMENTAL APPARATUS

III.1 Diode Laser System

A lead-salt semiconductor diode laser was used to obtain the high resolution spectra of $N_2$ quadrupole absorption lines. A semiconductor laser is a p-n junction device. When a n-type semiconductor is placed in contact with a p-type semiconductor, electrons from the n side will diffuse to the p side and holes from the p side will diffuse to the n side. The initially neutral n side, therefore, becomes positively charged and the initially neutral p side becomes negatively charged so that a field builds up to the point where a further flow of carriers is repelled. If an external voltage source is connected to oppose this equilibrium field (i.e., potential barrier), then the flow of electrons to the p side and holes to the n side will continue. The device is said to be forward biased. Semiconductor laser action is based on the fact that, at the p-n junction of a semiconductor diode that is forward biased, electrons and holes can recombine, with the emission of a photon occurring as well. A resonator can be formed by polishing the ends of the semiconductor or forming the ends by cleaving along natural crystal planes. The conditions for oscillation can thereby be met.

Just as electrons bound to an atom can have only discrete energy levels, so too electrons in a crystal can have only discrete energy
levels. However, because of interactions with the neighboring atoms in a crystal lattice these discrete levels lose their distinction and are grouped into bands. These bands are called the valence band, the forbidden band, and the conduction band. The allowed energy levels are closely spaced in the valence and conduction bands with a forbidden region between them. A typical semiconductor can have an energy separation (width of forbidden band) of from 0.01 to 4 electron volts (eV) while the separation between energy levels in the valence or conduction band may be $10^{-14}$ eV.

Laser action in semiconductors results from optical transitions across the energy gap (bandgap) between the nearly empty conduction band and the nearly full valence band. The emission photon energy is approximately equal to this bandgap energy. A diode laser is excited by applying a forward bias current and thereby injecting charge carriers (electrons or holes) across the p-n junction. The recombination of these injected minority carriers provides the gain mechanism for laser action. In operation the laser is cooled to a temperature of 50°K or less and subjected to a dc forward bias current greater than threshold. Threshold currents are typically between 100 and 500 mA. For the diode laser that was used, the threshold current was 258 mA at a temperature of 20°K.

A laser cavity can be operated in a variety of oscillation modes similar to those of a waveguide. As waves travel back and forth between the cleaved surfaces (which are essentially end mirrors) standing waves are set up when an integral multiple of half-wavelengths fits between the cleaved surfaces. In other words

$$\frac{L}{(\lambda/2)n} = m, \text{ or } mL = 2Ln$$

(82)
where \( m \) = an integer (axial mode number)  
\( \lambda \) = the wavelength in \( \mu \text{m} \)  
\( L \) = the length of the laser cavity,  
i.e., the distance between the cleaved surfaces  
and \( n \) = the refractive index of the medium at \( \lambda \)  

The spacing \( \Delta \lambda \) between these allowed spectral modes in the axial direction (direction defined by \( L \)) is the difference between the wavelengths defined by \( m \) and \( m + 1 \). Differentiating equation (82) with respect to \( \lambda \), yields:

\[
\frac{m \Delta \lambda + \lambda \Delta m}{\lambda^2 \Delta m} = \frac{2L \Delta n}{2L \Delta n - m \Delta \lambda} \tag{83}
\]

\[
\frac{\Delta \lambda}{\lambda^2 \Delta m} = -\frac{1}{2nL(1 - \lambda \frac{\Delta n}{\Delta \lambda})} \tag{88}
\]

In the limit as \( \Delta \lambda \to 0 \), \( \Delta n/\Delta \lambda \) can be replaced by the derivative \( dn/d\lambda \).  
Since \( \Delta m = 1 \) and \( \nu \) (in units of \( \text{cm}^{-1} \)) = \( 1/\lambda \) and \( \Delta \nu = -\Delta \lambda/\lambda^2 \), the spectral mode separation is given by

\[
\Delta \nu = +\frac{1}{2nL(1 - \lambda \frac{dn}{d\lambda})} \tag{89}
\]

Noting that

\[
\frac{dn}{d\lambda} = \frac{dn}{d\nu} \frac{d\nu}{d\lambda} = \frac{dn}{d\nu} \left(-\frac{1}{\lambda^2}\right) = \frac{dn}{d\nu} (-\nu^2) \tag{90}
\]

equation (89) can also be written as
The output emission for the lead-salt laser occurs in a series of narrow (0.0003 cm⁻¹) spectral modes separated in this case by about 3 cm⁻¹ as given by equation (89) or (91). Using equation (89) and \( n = 4.02, \frac{dn}{d\lambda} = -0.0118, L = 200 \mu m = 0.02 \text{ cm}, \) and \( \lambda = 4.134533 \mu m, \) the mode separation is computed to be 6.29 cm⁻¹. The values of \( n \) and \( \frac{dn}{d\lambda} \) are for germanium as given in Chapter IV. Using an index of 7.0 for a diode laser material such as PbS₃₋ₓSeₓ, and assuming a similar slope \( (\frac{dn}{d\lambda}) \), the mode separation is computed to be 3.5 cm⁻¹.

The above expression describing the spectral mode separation also results from a more rigorous derivation which starts with Maxwell's equations. The solution is obtained using separation of variables and the resulting expression contains Hermite-Gaussian functions. Using these functions, which comprise the electric field, and the boundary conditions, one obtains an expression for the resonant frequencies, which in turn will simplify to equation (91) when only axial modes are considered.

Coarse tuning of the laser over a typical range of 50-200 cm⁻¹ is accomplished by varying the temperature between 15°K and 100°K with typical tuning rates of 4 cm⁻¹/°K. Colder temperatures cause the laser to operate at longer wavelengths (smaller wavenumbers). Fine tuning over a maximum range of 1 cm⁻¹ is achieved by the small temperature changes induced by variations in the laser bias current. Increasing the bias current will cause the laser output to shift to shorter wavelengths (larger wavenumbers). These small changes in temperature affect the
refractive index of the semiconductor laser material, thereby altering the resonant frequencies of the Fabry-Perot laser cavity.

A Spectra-Physics, Laser Analytics Division, model SP5730 closed cycle refrigerator or cold head, serial number (S/N) 3918084, was used to house the laser diodes. Four mounting positions were available within the cold head. For the majority of the research, three diodes which lased in the 8-14 μm region were in positions 1 (S/N 4214-01), 2 (S/N 5109-29), and 3 (S/N 5108-03). A diode which lased in the 4.14-4.17 μm (2400-2415 cm⁻¹) region was specifically ordered to study the quadrupole transitions of N₂. This diode (S/N 8020-12) was made prior to the use by Laser Analytics of molecular beam epitaxy. It therefore took nine months by trial and error for Laser Analytics to fabricate a diode that both lased and lased in the correct spectral region. Initially this diode was installed into position 4. A week before data was collected on the quadrupole lines of N₂, this diode was moved to position 3, and diode S/N 5108-03 was removed. Into position 4 was placed a diode (S/N 8132-04) which was loaned to Ohio State University by Laser Analytics in the event that diode S/N 8020-12 did not operate properly during the final two weeks of experimentation, after which time the laboratory would not be available for N₂ studies. The diode originally ordered (S/N 8020-12) had indeed changed its properties, enough so that a sufficient signal to noise ratio could not be obtained in the S(8) region for a characterization of that line. However, the stability of the signal obtained using this diode proved to be better than the diode (S/N 8132-04) that was loaned to us.

The cold head was part of a three-component temperature-controlled refrigerator, the other two parts being a model SP5710 compressor and a
model SP5720 cryogenic temperature stabilizer. The compressor provided a closed cycle, high purity, pressurized (250 lbs/in² when running) supply of helium gas to the cryogenic refrigerator (cold head) via two 10-foot flexible lines. The temperature stabilizer automatically controlled and stabilized the temperature of the closed cycle refrigerator to user-set temperatures. The cold head was able to cool the laser diodes to 12°K, and the temperature within the cold head could be regulated to any user-set value within 0.002% over the range from 12 to 300°K. A model SP5820 laser control module allowed the user to select one of the four lasers, and provided the current and modulation control.

The diode laser is constructed using a stripe geometry, the stripe being 200 μm long but having a cross-section of only 10 μm x 10 μm. This stripe geometry is designed to suppress parasitic circulating and side-bounce emission modes and inhibit higher order transverse modes. However, the small cross-section is essentially the laser aperture and gives rise to a large divergence. Without a f/1 collimating lens, no long path absorption experiment would be possible with diode lasers. The spatial output pattern of the diode laser (S/N 8020-12) as it was emitted from the cold head, was found to have a divergence angle (full angle in any given plane) of 28°.

III.2 Detection Methods

The principal objective of this research was to characterize certain quadrupole absorption transitions in N₂. The way that these transitions were characterized was by measuring the transmission as a function of wavenumber. The energy of the transition will correspond to the line center of this curve (minimum transmission). The area enclosed by this
curve and the 100% transmission line will provide information on the integrated absorption or equivalent width of the absorption line, and the full-width-at-half-maximum value will shed light on the broadening mechanisms at work.

The usual approach to detecting a weak signal amidst a strong background is to modulate the laser beam and use a lock-in amplifier tuned to that modulation frequency. Scans taken in this way while sweeping the laser current (wavenumber) are called direct absorption scans. The noise that is present in these scans can be reduced by coadding many scans together. The noise level in the coadded result is then reduced over that of a single scan by a factor of $N^{-\frac{1}{2}}$ where $N$ is the number of scans.

A lock-in amplifier is basically a phase-sensitive detector which can be considered simply as a double-pole, double-throw reversing switch. The position of the switch is determined by the polarity of the reference input (modulation frequency). If the input signal from the detector is a noise-free sinusoid and if this signal is in phase with the reference signal (from the modulator), the output of the switch will be a full-wave rectified sinusoidal waveform. When filtered by a RC integrator, the output will be a dc level proportional to the rms value of the input signal. However, if the input and reference signals are out of phase with one another by 90° then the integrated output of the switch will be zero. Therefore the output of the lock-in amplifier is proportional to the rms value of the input signal and to the cosine of the phase angle between the input and reference signals\textsuperscript{48}.

The lock-in amplifier can be divided into four main sections: a signal channel, a reference channel, a mixer (the phase sensitive detector
mentioned earlier), and a dc amplifier/low-pass filter. In the signal channel, the input signal (and noise) is conditioned by the low-noise preamplifier and post-amplifier, with a filter sandwiched in between. The filter can be a tunable bandpass, notch, low- or high-pass network. The purpose of the filter is to reduce the possibility that the mixer will overload during severe noise conditions. The reference channel transforms the externally applied reference to a suitable square wave at the reference frequency to drive or switch the mixer. The output of the lock-in amplifier is independent of the reference amplitude as long as the reference exceeds a specified threshold, typically 100 mV.

Nonsynchronous inputs (noise) share no common frequencies with the reference and will not contribute dc components to the mixer output. When the mixer output is passed through the low-pass filter to remove ac fluctuations, the signal to noise (dc/ac) is enhanced in proportion to the square root of the filter time constant. The noise evident in the direct absorption scans are variations in the modulated signal, i.e., the laser output (temperature or vibrational instability) or variations (e.g. index of refraction) in the column of N₂ gas under study which cause small deviations in the laser beam path (beam wander).

Two alternative detection schemes (besides direct detection) used in this investigation include first harmonic detection and second harmonic detection (often called first and second derivative detection). These techniques take advantage of the fact that the lock-in amplifier can be made to lock onto either the fundamental of the reference frequency or one of its overtones. For harmonic detection, the mechanical chopper (modulator) is removed and in its place the drive current to the diode
laser is modulated by dithering the laser dc current at a frequency ≤ 10 kHz using circuitry which is part of the laser control module. This is done while the laser current is swept over the spectral range of interest. This modulation can also be provided by an external signal generator. In either case this modulation circuit is connected to the reference input on the lock-in amplifier, and for this work a frequency of 1 kHz was used. In the case of second harmonic detection, the lock-in amplifier is switched to 2f (i.e., twice the reference frequency).

Near the center of the molecular absorption line, a synchronously detected signal with f as the frequency of current modulation has an output which is approximately the first derivative of the absorption line profile. The use of this technique is very effective in enhancing small ac signals which change rapidly with wavenumbers while eliminating slowly varying background signals.

Figure 4 compares direct detection to first and second harmonic detection for a 1000 ppm sample of SO₂ in N₂ with 10 Torr total pressure and a path length of 40 m. Direct detection is plagued with strongly sloping background signals which are still evident in the first harmonic detection trace as a negative dc offset. This offset is proportional to the laser power incident on the detector. The position of the line center in a given absorption line is given by the peaks (minimas) in direct detection and second harmonic detection. The line center in the case of first harmonic detection is coincident with a zero crossing. Not shown in figure 4 is the noise usually present with each of these traces. Direct detection is the noisiest, while second harmonic detection has the least noise. The peak of the second harmonic signal can be used as a
Figure 4. Comparison of Direct Detection with First and Second Harmonic Detection
measure of the strength of the molecular absorption signal provided a calibration technique is used for each absorption line. In line position measurements, either the first or second harmonic technique can be used to locate the line center with improved accuracy over direct detection, since the location of the line center is sharper in the derivative signals than in the absorption signal. In linewidth measurements, the separation between the positive peak and the negative peak in first and second harmonic signals can be related to the linewidth of the absorption line provided the lineshape is known and the frequency deviation is kept very small. Second harmonic detection was used to detect the presence of the S(8), S(10), and S(12) lines of N₂ while direct detection was used to obtain transmission (absorption) versus wavelength (cm⁻¹) for the S(10) and S(12) lines. Even though the sensitivity of first and second harmonic detection to the presence of a line is better than direct detection by several orders of magnitude, the actual signal recorded is significantly smaller than that obtained with direct detection. Furthermore, the exact lineshape was not known and a measure of transmission versus wavelength was the primary goal. Integrating a second derivative (of transmission) signal twice to get transmission yields two unknown constants, while integrating a first derivative signal yields one unknown constant.

III.3 Detectors

Until the desired laser diode arrived, the cold head was operated with the diodes which lased in the 8-14 µm region. For this spectral region either a pair of Ge:Cu (copper-doped germanium) detectors (Spectra-Physics model SP 5750) or a pair of HgCdTe detectors (Santa Barbara Research Center or Infrared Associates, Inc.) were used to detect the
laser signal. The Ge:Cu detectors were mounted in a two-position cold head and cryogenically cooled in the same manner as the lasers. The HgCdTe detectors were in metal dewars and were cooled with liquid N\textsubscript{2}.

The spectral response of the Ge:Cu detectors was known to cover the 8-14 \(\mu\text{m}\) region. In fact, it covered the region from the visible to 30 \(\mu\text{m}\). The HgCdTe detectors, however, will detect radiation in either the 3-5 \(\mu\text{m}\) or 8-14 \(\mu\text{m}\) or both, depending on the stoichiometric ratios of Hg: Cd:Te. The relative spectral responses of the HgCdTe detectors were determined using an IBM IR98 Fourier transform spectrometer. A DTGS (deuterated triglycine sulfate) pyroelectric detector was used as a reference because pyroelectric detectors have reasonably flat response curves with respect to wavelength. The relative spectral response for the Santa Barbara Research Center (SBRC) HgCdTe detectors, S/N 4137 and S/N 4138 were found to be sensitive to radiation in the 3-5 \(\mu\text{m}\) region.

After receiving laser diode S/N 8020-12, the Ge:Cu detectors were put aside in favor of liquid-N\textsubscript{2}-cooled InSb detectors. The motion of the piston in the cold head on the Ge:Cu detectors added noise to the signal, and InSb detectors have higher responsivities in the 3-5 \(\mu\text{m}\) than Ge:Cu detectors. The particular InSb detectors used were both Infrared Associates, Inc., with serial numbers I-419-IS and G-198-IS R.

### III.4 Twenty-Two-Meter White Cell

Three White (multi-pass) cells were evaluated and/or put into function. Prior to obtaining the equipment from NOAA, the reflectance of the mirrors in the 22 m-base-length fiberglass cell at Denison University was measured. It was anticipated that, if sufficiently long paths could not be obtained with other shorter cells, the experiment to study N\textsubscript{2} would
be relocated to Denison University. Path lengths of several kilometers have been achieved with the 22 m cell.

It was assumed that the three mirrors of this White cell were of the same radius of curvature and reflectance. Mirrors for White cells are usually ground from the same piece of glass, cut into three parts, and then coated. If the sputtering chamber is large enough, the three mirrors are coated simultaneously.

The reflectance of these mirrors at a given wavelength can be derived from a measurement of the intensity exiting the cell after n reflections as a function n. If $I_0$ is the intensity of the source prior to entering the cell, $I_1$ is the remaining intensity after one reflection, $I_2$ after two reflections, ..., $I_n$ after n reflections, and r is the reflectance, then

$$I_1 = I_0 r$$  \hfill (92)

and

$$I_2 = I_1 r = (I_0 r) r = I_0 r^2$$  \hfill (93)

One can deduce from this that

$$I_n = I_0 r^n$$  \hfill (94)

Rearranging equation (94) and taking the logarithm, equation (94) becomes

$$\log_{10}(I_n/I_0) = n \log_{10}(r)$$  \hfill (95)

If $\log_{10}(I_n/I_0)$ is plotted on the y-axis and n on the x-axis, the slope of this straight line will be $\log_{10}(r)$.

The reflectance was measured at three wavelengths: 0.6328 μm, 2.09 μm, and 3.67 μm. A 35 mW helium-neon (HeNe) laser was used for 0.6328 μm, and a tungsten-halogen lamp with filters was used as a source for the other two wavelengths. As shown in figure 5, a portion of the HeNe laser beam was diverted towards a silicon detector with a neutral density filter.
Figure 5. Experimental Set-up Used at Dension to Measure Reflectance
positioned at 45° to the beam. Before detecting this reference intensity, a second neutral density filter was needed before the silicon detector. A second silicon detector was positioned to receive the laser beam after passing through the cell.

The output of the reference detector was connected to a Princeton Applied Research (PAR) model HR-8 lock-in amplifier and the output of the detector for the cell was connected to a PAR model 5207 lock-in amplifier. A PAR 192 variable speed chopper operating at 555.6 Hz was positioned after the laser. The TTL output from the chopper was used as a reference signal for the lock-in amplifiers. Outputs from the lock-in amplifiers were input to a Hewlett-Packard (HP) 3456A ratiometer.

The number of passes through the cell can be determined from the number of images seen on the single mirror in the cell at the end of the cell nearest the input and output windows. The number of passes, $p$, is two times the number of images, $i$, plus two, or

$$p = 2i + 2 \quad (96)$$

The number of reflections, $n$, would be one less than the number of passes, or

$$n = 2i + 1 \quad (97)$$

The path length would be the number of passes times the base length of the cell. The resulting data for 0.6328 μm are given in Table 2. A least squares calculation for the slope yielded a reflectance of 97.60%.

Referring to figure 5, the 35 mW HeNe laser was replaced with a tungsten-halogen lamp. A filter wheel was constructed and positioned after the chopper. A Cleartran® (water-clear ZnS) window was used as a beam-splitter. Three CaF$_2$ lenses were needed; one to ensure that the infrared
beam was focused soon after it entered the cell, one to further focus the portion of the beam split off for the reference detector, and one to focus the beam onto the second detector after it left the cell. The silicon detectors were replaced with two liquid-nitrogen-cooled InSb detectors.

The InSb detectors were both Infrared Associates detectors, serial numbered I-419-IS for the reference, and G-198-IS R for the cell. An Acopian K20D50 dual power supply was used to provide power to the detector preamplifiers. The same lock-in amplifiers and ratiometer were used as before.

A beamsplitter cube was kinematically mounted between the cell and the second detector to facilitate alignment of the optics for the infrared measurements. A smaller HeNe alignment laser was then both reflected back to the second detector and into the cell by the cube. The cube was removed prior to collecting reflectance data.

Table 3 contains the data collected for the two wavelengths in the infrared. The least squares calculations on the data gave 98.49% for 2.09 \( \mu m \) and 97.16% for 3.67 \( \mu m \).

III.5 Four-Meter White Cell

After measuring the reflectance of the mirrors in the 22 m cell at Denison, a 4 m-base-length stainless steel cell was obtained from NOAA. Remote controls were added to the end of the cell which housed the pair of D-shaped mirrors. A total of six controls were added. Each mirror had a micrometer screw for rotation on the rear surface of the mirror located midway in height and at the edge of the mirror nearest the outside of the cell, and two coarse tilt adjustments on the opposite side of the rear surface, one near the bottom and one near the top of the mirror.
Six holes were drilled in the rear steel plate of the cell so that rods could be connected to the mirror adjustments. Cajon Ultra-Torr male connectors, part number B-4-UT-1-4 were adapted for use as Wilson seals around the rods inserted in the holes. A 0.25" diameter aluminum rod was then inserted into each of the six Wilson seals. On the end of each rod intended for coarse tilt adjustments (4 in all) was attached a universal joint. The other side of each universal joint was attached to an allen key segment which in turn fit into the corresponding head of the allen bolt tilt adjustment on the mirror. The two aluminum rods for controlling the micrometer rotation adjustments were attached to the micrometers with two sizes of rubber tubing and one hose clamp. Large plastic disk handles, as taken from common valve fixtures were attached to the ends of the aluminum rods which extended to the outside of the 4 m cell.

A 2.0 inch diameter Plexiglas® window was added to the rear steel plate, above the controls for the mirrors to allow viewing into and along the axis of the cell. A 6X telescope was fabricated and clamped into position at the Plexiglas® window. The number of images on the single mirror at the other end of the cell, produced using a helium-neon laser as the source, could then be visually counted.

An oscilloscope was positioned at the end of the cell with the remote controls. This scope displayed the signal to the lock-in amplifier. This scope was especially useful for determining the number of infrared images, as the signal would go to zero between one set of images and the next.

It was then determined that the mount for the input window to the 4 m cell was in the wrong position. The single mirror at the input/output end of the cell occluded the input beam. The input window mount
was shifted by 0.375".

Two MKS Baratron pressure heads, one 10 Torr and one 1000 Torr head, were connected to the cell via a soldered network of rigid copper tubing. The heads were connected through a 'T' joint, and a single line of tubing then connected the 'T' to the cell. The heads were electrically connected to a MKS Baratron model 170M-34B head selector, model 170M-27C digital readout, and model 170M-6B range multiplier.

The reflectance of the mirrors in the 4 m cell was then measured in the same way as for the 22 m cell described earlier. A least squares fit to the data in Table 4 yielded reflectances of 95.78% and 96.34% for 0.6328 µm and 4.15375 µm, respectively.

Up to this point the maximum useable path length achievable with the 4 m cell at 4.2 µm was 160 m to 200 m. A corner cube was added bringing the maximum path length to 408 m. The corner cube consisted of two one-inch-diameter plane mirrors each attached to a Newport Corporation MM-1 mirror mounts as shown in figure 6. These two mounts were in turn attached with bolts to vertical slots in a piece of aluminum. The slots allowed the distance between the mirrors to be adjusted which determined the distance between rows of images. This aluminum together with the two mirrors and MM-1 mounts was attached to the side of the single 4 m ROC mirror (input/output end) mount by drilling and tapping two holes. With the addition of this corner cube, the output beam no longer passed out the output window. It exited below the input beam. Two additional flat mirrors were installed in the 4 m cell behind the single mirror to reflect the output beam back to the output side and to reflect the output beam out of the output window.
Figure 6. Side View of Retroreflector Assembly
A type T (copper-constantan) thermocouple was installed in a small port on one side of the cell and connected to a Fluke 2190A thermocouple voltmeter and a Joseph Kaye Company, Inc. model RCS4 ice point reference. In particular two thermocouple junctions were heli-arc welded (using argon gas) to allow the use of an ice bath reference. This double thermocouple consisted of a seven-foot-length of copper, joined at the first junction to a four-foot-length of constantan. The other end of this constantan was connected via the second junction to a three-foot-length of copper. The two copper ends were fastened to the Fluke, the first junction epoxied into the cell, and the second junction inserted into the ice point reference. See figure 7. The Fluke was made to operate in the voltmeter mode to bypass internal electronic reference junctions which are used by the Fluke to convert voltages to temperatures.

Copper tubing (0.25") was made into 12" diameter coils and then soldered to the outside of a sheet of 16 oz./ft² copper which had been bent into the shape of a cylinder. Three 32" long sections were made and then installed into the 4 m cell through the end containing the input/output windows. After the first section was in the cell, the tubing of the second section was soldered to the tubing of the first. These two sections were pushed into the cell further and the third section attached to the second. Two small ports on top of the cell, which originally were equipped with thermocouples, were used to allow the entry and exit of the tubing ends. Liquid N₂ was tried as a refrigerant to get the N₂ gas in the cell down to 157°K and increase the number density by nearly a factor of 1.4. Using the ideal gas law with constant pressure and volume, this factor of 1.4 arises from the ratio of the before and after temperatures,
Figure 7. Thermocouple Wiring Diagram
### TABLE 2

**MEASURED INTENSITY RATIOS VS. NUMBER OF REFLECTIONS FOR THE 22 m CELL AT 0.633 μm**

<table>
<thead>
<tr>
<th>IMAGES REFLECTIONS</th>
<th>PASSES</th>
<th>PATH LENGTH</th>
<th>( \frac{I_n}{I_0} )</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>3</td>
<td>4</td>
<td>88 m</td>
</tr>
<tr>
<td>3</td>
<td>7</td>
<td>8</td>
<td>176 m</td>
</tr>
<tr>
<td>5</td>
<td>11</td>
<td>12</td>
<td>264 m</td>
</tr>
<tr>
<td>7</td>
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<td>9</td>
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<td>20</td>
<td>440 m</td>
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<td>11</td>
<td>23</td>
<td>24</td>
<td>528 m</td>
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<td>13</td>
<td>27</td>
<td>28</td>
<td>616 m</td>
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<td>704 m</td>
</tr>
<tr>
<td>17</td>
<td>35</td>
<td>36</td>
<td>792 m</td>
</tr>
<tr>
<td>19</td>
<td>39</td>
<td>40</td>
<td>880 m</td>
</tr>
<tr>
<td>21</td>
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<td>1496 m</td>
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<tr>
<td>35</td>
<td>71</td>
<td>72</td>
<td>1584 m</td>
</tr>
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</table>

### TABLE 3

**MEASURED INTENSITY RATIOS VS. NUMBER OF REFLECTIONS FOR THE 22 m CELL AT 2.09 μm AND 3.67 μm**

<table>
<thead>
<tr>
<th>IMAGES REFLECTIONS</th>
<th>( \frac{I_n}{I_0}(2.09 , \mu m) )</th>
<th>( \frac{I_n}{I_0}(3.67 , \mu m) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>2.20</td>
<td>0.212</td>
</tr>
<tr>
<td>13</td>
<td>1.96</td>
<td>0.189</td>
</tr>
<tr>
<td>15</td>
<td>1.75</td>
<td>0.169</td>
</tr>
<tr>
<td>17</td>
<td>1.51</td>
<td>0.148</td>
</tr>
<tr>
<td>19</td>
<td>1.45</td>
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</tr>
<tr>
<td>21</td>
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<tr>
<td>27</td>
<td>0.758</td>
<td>0.078</td>
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</table>
### TABLE 4

**MEASURED INTENSITY RATIOS VS. NUMBER OF REFLECTIONS FOR THE 4 m CELL AT 0.6328 μm AND 4.15375 μm**

<table>
<thead>
<tr>
<th>IMAGES</th>
<th>REFLECTIONS</th>
<th>PASSES</th>
<th>PATH (m)</th>
<th>$I_n/I_0$ (0.6328 μm)</th>
<th>$I_n/I_0$ (4.15375 μm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3</td>
<td>4</td>
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<td>0.05641</td>
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<td>3</td>
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<td>0.321306</td>
</tr>
<tr>
<td>5</td>
<td>11</td>
<td>12</td>
<td>48</td>
<td>0.02036</td>
<td>0.300000</td>
</tr>
<tr>
<td>7</td>
<td>15</td>
<td>16</td>
<td>64</td>
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</tr>
<tr>
<td>9</td>
<td>19</td>
<td>20</td>
<td>80</td>
<td>0.00774</td>
<td>0.271034</td>
</tr>
<tr>
<td>11</td>
<td>23</td>
<td>24</td>
<td>96</td>
<td>0.00552</td>
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<td>28</td>
<td>112</td>
<td>0.00318</td>
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</tr>
<tr>
<td>15</td>
<td>31</td>
<td>32</td>
<td>128</td>
<td>0.0017719</td>
<td>0.230345</td>
</tr>
<tr>
<td>17</td>
<td>35</td>
<td>36</td>
<td>144</td>
<td>0.0011168</td>
<td>0.208966</td>
</tr>
<tr>
<td>19</td>
<td>39</td>
<td>40</td>
<td>160</td>
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</tr>
<tr>
<td>21</td>
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<td>44</td>
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<td>0.095890</td>
</tr>
<tr>
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<td>48</td>
<td>192</td>
<td>0.0001507</td>
<td>0.031507</td>
</tr>
</tbody>
</table>

multiplied by the ratio of the Boltzmann factors and the ratio of the partition functions. After five hours of pouring liquid N$_2$ into the coils, an equilibrium temperature of 280°K was reached. The liquid N$_2$ was replaced with methyl alcohol and the alcohol was circulated and cooled using a Lauda closed cycle cooler capable of cooling to 143°K. Again 278-280°K was the lowest attainable temperature. Four layers of thin foam insulation were wrapped around the length of the cell. A temperature of 273°K was reached. Temperature gradients due to the lack of insulation at the ends of the cell produced a changing index of refraction. This in turn caused the laser beam to wander giving an erratic signal on the lock-in amplifier.

III.6 Ten-Meter White Cell

A ten-meter-long steel White cell was made functional in order to gain a factor of 2.5 in path length over that achievable with the four-meter cell. Two 6.0-inch-square gold-coated mirrors were mounted in the
north end of the cell, and a 4.0 by 12.0 inch gold-coated mirror was positioned in the south end. All three of these mirrors had a radius of curvature of 10 m.

Several changes were made to the half-finished mirror mounts in an attempt to facilitate the changing of path length and to ensure that the image pattern obtained would not change once established. The mirror mount had to be redesigned to pivot on a single ball bearing for rotation and about two ball bearings for tilt. Both adjustments were accomplished with micrometer screws. Brass adaptor rods were machined so that 0.25-inch rods could be connected to the micrometer screws. The 0.25-inch rods were made long enough to extend from the mirror micrometer screws to the White cell end plate and through Wilson seals in the plate. Prior to machining the end plate to receive the Wilson seals, the experiment was moved to Denison University to use the 22 m White cell.

III.7 Monochromators for Sorting Modes

The laser diode emitted two strong modes, and at least one weaker mode. The number of modes and the relative strengths of these modes varied with the temperature of the diode laser. As mentioned in section III.1, these modes are 2 to 3 cm\(^{-1}\) apart, and all would be detected by the InSb detectors unless some filtering were done. For the 4 m and 10 m White cells at Ohio State University, the optical layout was such to allow the beam to pass through either a grating monochromator, or an echelle spectrograph to allow only one mode to continue on to the White cell and to provide some coarse indication of the spectral range. For the work at Denison University, only the grating monochromator was aligned with the system.
The calibration for each of these monochromators is discussed in Chapter IV. It was found, though, after calibrating the echelle spectrograph that the extremely high dispersion it offered diminished the laser signal to a nearly undetectable level.

III.8 Interface Circuits

Prior to realizing that the echelle spectrograph would not be used, a position sensor circuit was designed and fabricated which would indicate to the computer data acquisition system (see Chapter V) increments in the dial setting of the echelle. This circuit was added to existing circuitry for rotating the echelle. The output of this position sensor circuit was a transistor-transistor-logic five volt pulse. Two pulses were emitted per dial number increment. This signal was connected with BNC cable to a digital input module of the computer system.

Another circuit, consisting of a system of relays, was devised to allow the echelle motion control circuits to be activated by the computer via a digital output module. Without a shaft encoder or other means to determine the absolute value of the echelle dial number, the beginning and ending positions were obtained through software prompts.

III.9 Optical and Electronic Layouts

A corner cube assembly similar to that shown in figure 6 was constructed for the 10 m cell to double the path length to a maximum of 1.4 km. The internal optical layout of the 10 m cell before and after the corner cube was added is given in figure 8.

Normally, on the single mirror in a White cell (nearest the input/output windows) can be seen two horizontal rows of images. Referring to the normal configuration of figure 8, the incident beam enters the input
NORMAL WHITE-CELL CONFIGURATION

A, B, C are Spherical Mirrors each of 10m Radius of Curvature.

DOUBLED PATH LENGTH WHITE-CELL CONFIGURATION

D, E are Plane Mirrors.

Figure 8. Internal Optical Layout of 10 m White Cell Before and After Adding A Retroreflector Assembly
window and is made to come to a focus using large f/number optics as it passes the front surface of the single mirror. The beam expands as it traverses the length of the cell until it encounters one of the pair of mirrors at the other end. This mirror refocuses the beam back onto the single mirror at the lower left-hand corner when looking directly at this mirror (labelled "1" in figure 9). This image is reflected from the single mirror towards the second of the pair of mirrors at the other end. This expanded beam is again refocused onto the single mirror but the image is located in the upper right-hand corner (labelled "2" in figure 9). This process is repeated with the next image at the lower left-hand corner but closer to the center of the single mirror, and the fourth image in the upper right-hand corner, also closer to the center of the mirror. Images are added in succession until an image in the bottom row falls off the right side of the single mirror, and an image in the top row falls off the left side of the single mirror. The image in the top row passes through the output window to the detector and this image is at the same height as the input beam.

In the case of the 10 m cell without the corner cube, there were two rows of images, and with the corner cube there were four rows of images. However, in the case of the 22 m cell, two corner cube assemblies were installed resulting in six rows of images. This is depicted in the photograph of figure 10 for a path length of 3.96 km using a helium-neon laser.

The optical layout and signal processing network used for the collection of data at Denison University are given in figures 11 and 12. The networks used for the 4 m and 10 m cells were essentially the same
Figure 9. White Cell Image Pattern
Figure 10. Photograph of Images On the 22 m White Cell Mirror for A Path Length of 3.96 km
Figure 11. Optical Layout Used with the 22 m White Cell
Figure 12. Electronic Layout Used with the 22 m White Cell
apart from the computer system that was used.

III.10 Vibration Isolation

Some consideration was given to vibration isolation because the cycle of the cold head refrigerator piston (3 Hz) was the major source of signal variation. Even though lock-in amplifiers were used which would normally filter out the 3 Hz component, the motion of the laser diode and detectors (in the case of the Ge:Cu detectors) caused the signal to vary because all of the optical components and alignment were fixed while the laser and/or detectors moved up and down. The amplitude of the motion, however small, was greatly magnified due to the fact that the active area of the laser was only 10 by 10 μm (i.e., the laser had a large divergence) and that long optical paths were being used.

In order to circumvent this problem, Sams and Fried\textsuperscript{49} fastened a microphone to a cold head and designed a microphone triggering circuit which would allow data collection during relatively short and quiet portions of the piston cycle. They found that the mechanically induced frequency-jitter can be as high as 40 kHz. This technique, however, precludes the use of a lock-in amplifier, which in turn makes it difficult to separate a weak signal from a strong background. Thirty thousand scans were required in Sams and Fried's work using sweep integration and coaddition of scans.

This technique was not considered for N\textsubscript{2} because it was found that the laser temperature varied sufficiently from scan to scan to warrant adjustments to each scan prior to coadding them. A discussion of the corrections which had to be made to each N\textsubscript{2} scan for temperature drifts is given in Chapter VII.
The vibration was finally isolated to motion in the collimating lens which is mounted one inch in front of the laser diode. Two different mounts were machined and attached to various translation and rotation stages. Both of these were found to be ineffective in reducing the vibration. A Newport Corporation LP-1-XYZ mount when clamped to the optical table reduced the vibration to a tolerable level, when used in conjunction with large c-clamps to hold down the cold head.
IV.1 Echelle Spectrograph at OSU

An echelle spectrograph was to be used as the order sorter and coarse filter for the diode laser. The spectrograph was located between the 4 m and 10 m White cells at OSU and would have provided higher spectral resolution than the grating provided with the diode laser spectrometer. In order to obtain a relationship between the dial number on the spectrograph and wavelength, the echelle spectrograph was calibrated as described below.

A helium-neon (HeNe) laser, a Hg arc lamp, and a Laakman RF-44 4 W waveguide CO₂ laser were used as sources, each in turn focused onto the entrance slit of the spectrograph. The collimating and collecting mirrors both had focal lengths of 2 m and were about 24.8 cm in diameter. The 31 groove/mm echelle was 20 cm by 30 cm and was positioned at a steep angle with respect to the beam incident upon it from the collimating mirror.

The CO₂ laser was directed through a piece of ZnS at 45° to a beam stop, so that most of the 4W would be dissipated. The five percent or so reflected from the ZnS was directed to the input slit of the echelle monochromator. The CO₂ laser required water cooling so that the length of the waveguide would remain constant, which in turn would ensure that the output wavelength did not change. A Lauda K75-DW closed cycle cooler was connected to the laser using methyl alcohol as the refrigerant. The
Lauda cooler maintained the temperature of the alcohol to within ± 0.02°C of the selected temperature.

With the exit slits nearly closed, it was possible to see the helium-neon and the Hg arc lamp images emerging from the slits. A silicon photodiode was used however to obtain the exact maxima of the visible images as a function of dial number.

Thermal printer paper was used to align the CO₂ laser beam with the input slits of the monochromator, but the emerging signal was too weak to burn the paper at the exit slit. A Ge:Cu detector cooled to 15°K was used to detect the emerging beam.

The resulting data points are given in Table 5, and the calculated least squares fit to the data using selected points yielded a slope of -461.198 dial numbers/cm⁻¹, and an intercept of 237869.5 dial numbers. The fit was done for an ordinate of dial numbers, and an abscissa of first order wavenumbers.

IV.2 Laser Analytics Grating Monochromator

The grating monochromator which was part of the laser diode system was used for the N₂ scans and was calibrated in a manner similar to that of the echelle. Only HeNe and Hg green were used as sources. The resulting plot is given in figure 13. The calibration of this monochromator covered a larger spectral region, thus showing the true curvature of the grating equation. The data points obtained in this calibration are given in Table 6. A least squares fit was done using the last two HeNe points, i.e., the 26th and 27th orders, yielding a slope of -0.06991 cm⁻¹/dial number and an intercept of 1195.7165 cm⁻¹. This equa-
### TABLE 5
DATA POINTS FOR ECHELLE CALIBRATION

<table>
<thead>
<tr>
<th>SOURCE</th>
<th>WAVELENGTH</th>
<th>DIAL NUMBERS</th>
</tr>
</thead>
<tbody>
<tr>
<td>HeNe</td>
<td>0.6328 μm</td>
<td>46171, 40696, 35518.5, 30619</td>
</tr>
<tr>
<td>Hg Arc</td>
<td>Green</td>
<td>45250.5, 40563, 40538</td>
</tr>
<tr>
<td></td>
<td>(0.5461 μm)</td>
<td></td>
</tr>
<tr>
<td>Hg Arc</td>
<td>Violet</td>
<td>43776, 43804, 42797, 42779, 40097, 40067</td>
</tr>
<tr>
<td></td>
<td>(0.4047, 0.4358 μm)</td>
<td></td>
</tr>
<tr>
<td>Hg Arc</td>
<td>Yellow</td>
<td>43030, 42265, 38179, 37440</td>
</tr>
<tr>
<td></td>
<td>(0.5770, 0.5790 μm)</td>
<td></td>
</tr>
<tr>
<td>CO₂</td>
<td>10.61 μm</td>
<td>20546</td>
</tr>
<tr>
<td></td>
<td>10.59 μm</td>
<td>19915</td>
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<td>10.55 μm</td>
<td>19304</td>
</tr>
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<td></td>
<td>10.53 μm</td>
<td>18713</td>
</tr>
<tr>
<td></td>
<td>10.51 μm</td>
<td>18432</td>
</tr>
</tbody>
</table>

The method was used to determine the approximate dial numbers corresponding to the locations of the quadrupole $N_2$ lines. For example, the wavenumber position of the S(8) line is 2403.5685 cm$^{-1}$. Since the grating was being used in 4th order, the first order wavenumber was 600.89 cm$^{-1}$. Using the slope and intercept mentioned above, the dial number was found to be 8508.85. During the collection of data, i.e., between scans, the collimating lens in front of the laser was adjusted to obtain a more stable signal and to improve the alignment. These adjustments change the angle with which the laser beam enters the monochromator, which in turn alters the calibration. It was found, by comparison with the positions of the $N_2O$ absorption lines, that this calculated dial number had to be systematically offset by -4.2683. In other words, the optimum position for the S(8) line was at a dial number of 8504.53.
Figure 13. Calibration Curve for the Grating Monochromator
<table>
<thead>
<tr>
<th>GRATING ORDER</th>
<th>WAVE NUMBER (cm⁻¹)</th>
<th>DIAL</th>
<th>GRATING ORDER</th>
<th>WAVE NUMBER (cm⁻¹)</th>
<th>DIAL</th>
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<td>1128.77</td>
<td>4539.6</td>
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<td>1053.52</td>
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<td>987.67</td>
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<td>25</td>
<td>632.11</td>
<td>8087.7</td>
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HG ARC GREEN

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<th>DIAL</th>
<th>GRATING ORDER</th>
<th>WAVE NUMBER (cm⁻¹)</th>
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<td>16</td>
<td>1144.48</td>
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<td>2247.6</td>
<td>23</td>
<td>796.16</td>
<td>6425.4</td>
</tr>
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<td>29</td>
<td>631.44</td>
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</table>
IV.3 Germanium Etalon

A 2.54-cm-long solid germanium etalon (Laser Analytics LOA-001) was used to provide the relative scale in wavenumbers for the N\textsubscript{2} scans by inserting the etalon into the beam before each set of N\textsubscript{2} scans and sweeping the laser current over the same region to be used for the N\textsubscript{2} scans. The fringe spacing, $\Delta \nu$, is nominally 0.048 cm\textsuperscript{-1} at room temperature and pressure and is given by equation (89).

The length of the etalon was carefully measured and found to be 1.01608 ± 0.00002 inches, or, multiplying by 2.54 cm/inch, 2.5808432 ± 0.00000508 cm. The index of refraction was computed using the following polynomial expression

$$n(\lambda) = A + BL + CL^2 + DL^3 + EL^4$$

(98)

where $L = 1/(\lambda^2 - 0.028)$, $A = 3.99931$, $B = 3.91707 \times 10^{-1}$, $C = 1.63492 \times 10^{-1}$, $D = -6.0 \times 10^{-8}$, and $E = 5.3 \times 10^{-8}$. The values of $n(\lambda)$ computed using (98) have uncertainties of ±3 $\times$ 10\textsuperscript{-4} or less, when compared to measured values of the index. The derivative $dn/d\lambda$ was found by fitting a straight line to the log-log plot of the absolute value of $dn/d\lambda$ versus $\lambda$ for germanium as given in The Infrared Handbook\textsuperscript{51}. The resultant least squares expression was found to be

$$\frac{dn}{d\lambda} = 1.491 \lambda^{-3.4906}$$

(99)

with a residual (difference between the actual and calculated $dn/d\lambda$ value) of 9.6 $\times$ 10\textsuperscript{-4} at 4.0 $\mu$m. The actual value of $dn/d\lambda$ is -1 times the result obtained using equation (99). For the S(10) and S(12) lines of N\textsubscript{2}, the fringe spacing was computed using the measured length and equations (89), (98) and (99). For the S(10) line, $\Delta \nu = 0.047644 \pm 0.000046$ cm\textsuperscript{-1}/fringe,
and for the $S(12)$ line, $\Delta \nu = 0.047633 \pm 0.000047$ cm$^{-1}$/fringe.

The uncertainty in these etalon spacing values was determined using the law of propagation of errors. Given a function $f = f(x_1, x_2, x_3, \ldots, x_n)$, the most probable error in $f$, or $\Delta_p f$, is given by

$$\Delta_p f = \sqrt{\sum \left(\frac{\partial f}{\partial x_i}\right)^2 (\Delta x_i)^2}$$

For multiplication (e.g., conversion from inches to centimeters as was done for $L$), if $M = xy$, then using equation (100), the most probable error in $M$ is $\Delta_p M = \sqrt{y^2 (\Delta x)^2 + x^2 (\Delta y)^2}$. For the example given, $x = 2.54$, $\Delta x = 0.0$, $y = 1.01608$, and $\Delta y = 0.00002$. For division, if $D = x/y$, then the most probable error in $D$ is $\Delta_p D = \sqrt{\frac{(\Delta x)^2}{y^2} + \frac{x^2 (\Delta y)^2}{y^4}}$. This simple formula was needed to convert from $\nu$ to $\lambda$. The wavelength in $\mu$m corresponding to $\nu = (2418.6526 \pm 0.003)$ cm$^{-1}$ was obtained from $\lambda = \frac{1 \times 10^4}{2418.6526}$. In this case $x = 1 \times 10^4$, $\Delta x = 0.0$, $y = 2418.6526$ for the $S(10)$ line, and $\Delta y = 0.00003$. This wavelength was found to be $(4.134533 \pm 0.000005) \mu$m. Similarly, the wavelength for the $S(12)$ line was found to be $(4.109157 \pm 0.000005) \mu$m.

Using $\Delta \nu$ from equation (89) as $f$, the most probable error in $\Delta \nu$, or $\Delta_p (\Delta \nu)$, is given by equation (100) as

$$\Delta_p (\Delta \nu) = \sqrt{4L^2 (\Delta \nu)^4 (\Delta n)^2 + \lambda^2 \left(\frac{dn}{d\lambda}\right)^2 (\Delta \lambda)^2 + (\Delta \nu)^2 \left(\frac{dL}{d\lambda}\right)^2}$$

Using equation (98), the indices of refraction were found to be $4.0227 \pm 0.0003$ and $4.0230 \pm 0.0003$ for the $S(10)$ and $S(12)$ lines, respectively. Using equation (99), the derivatives of the index were computed to be $-0.01053 \pm 0.00096$ and $-0.01076 \pm 0.00096$ for the $S(10)$ and $S(12)$ lines,
respectively.

The wavenumber spacing for a given set of N₂ scans was determined from the etalon scan taken prior to those scans by graphically determining the spacing (in units of laser current) between etalon fringes. This gave a conversion factor in terms of amperes/fringe. Dividing the computed fringe spacing by this conversion factor gave an etalon tuning rate in units of cm⁻¹/ampere.

The uncertainty in the etalon tuning rate for a given N₂ line depended upon the uncertainties associated with 1) determining the location, graphically, of the first and last peak in the etalon scan, i.e., obtaining two laser current values; 2) computing the difference and dividing the result by the number of fringes (usually six to nine fringes were observed.); and 3) dividing this result into the previously computed value of the etalon tuning rate, which was in units of cm⁻¹/fringe, to convert the tuning rate into units of cm⁻¹/ampere.

In one case (S(12) at 729 Torr), for step (1), the midpoint of two laser current values was used to locate each peak. This was done because the etalon peak was distorted or flat. Two points with the same y value were chosen below the peak, where the fringe became more symmetrical.

The uncertainties associated with the graphical determination of the laser current values were ± ½ the smallest division that was used. Generally these were values on the order of microamperes. These errors were then combined using equation (100) for the subtraction of two quantities. If \( S = x - y \), then \( \Delta_p S = [(\Delta x)^2 + (\Delta y)^2]^{1/2} \). For the S(12) data at 729 Torr, two values were averaged to obtain x, and two values were averaged to obtain y. Prior to combining the errors to obtain the
uncertainty in $S$ in this case, the error in $x$ or $y$ was computed using equation (100) for addition and division. The formula for addition is identical to that derived for subtraction. In computing the average, the divisor is 2 and it has zero uncertainty. The formula for division ($D = x/y$) then simplifies to $\Delta_p D = \Delta x/y$. At this point the computed errors are associated with the amperes/fringe values.

The uncertainty associated with step (3), i.e., the division of the cm$^{-1}$/fringe values by the amperes/fringe values, was again determined using equation (100) solved for division, and using the uncertainties previously computed. The resulting uncertainties were due primarily to the errors in the cm$^{-1}$/fringe values. These resulting etalon tuning rates and their uncertainties in units of cm$^{-1}$/ampere are given in Table 7.

**TABLE 7**

<table>
<thead>
<tr>
<th>$N_2$ Line</th>
<th>Pressure (Torr)</th>
<th>Etalon Tuning Rate (cm$^{-1}$/ampere)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S(10)</td>
<td>730</td>
<td>11.4548 ± 0.0117</td>
</tr>
<tr>
<td>S(10)</td>
<td>734</td>
<td>11.5655 ± 0.0115</td>
</tr>
<tr>
<td>S(10)</td>
<td>837</td>
<td>11.7243 ± 0.0116</td>
</tr>
<tr>
<td>S(12)</td>
<td>729</td>
<td>14.9470 ± 0.0147</td>
</tr>
<tr>
<td>S(12)</td>
<td>732</td>
<td>14.9456 ± 0.0148</td>
</tr>
<tr>
<td>S(12)</td>
<td>837</td>
<td>14.3296 ± 0.0142</td>
</tr>
<tr>
<td>S(12)</td>
<td>880</td>
<td>14.8788 ± 0.0147</td>
</tr>
<tr>
<td>S(12)</td>
<td>950</td>
<td>15.0248 ± 0.0150</td>
</tr>
</tbody>
</table>

Due to the size of the input aperture of the etalon ($\approx$ 1 cm), it had to be placed between the laser and the 2.5X beam expander. The etalon was mounted in a v-block tip-and-tilt stage, which in turn was mounted to four posts. These posts were attached to machined strips of aluminum. Mechanical stops were then mounted to the optical table against the metal strips of the etalon mount after the etalon was aligned with the beam.
These stops facilitated the kinematic repositioning of the etalon from one set of N₂ scans to the next.

IV.4 N₂O Calibration Cells

Two calibration cells containing N₂O were used during data collection; a large (50.5 cm) and a small (16 cm) cell. The large cell was inserted into the laser beam path and scanned prior to taking a set of 20 scans on the White cell, while the small cell was permanently positioned to receive a portion of the laser power diverted to it with a CaF₂ beam-splitter.

The large cell had previously been filled with a low pressure of NH₃. It was evacuated using roughing and diffusion pumps and then backfilled with helium gas. This procedure was repeated several times. The helium gas helped to dislodge the tenacious NH₃ molecules from the walls of the cell. Figure 14 is a drawing of the plumbing arrangement for evacuating the cell and backfilling the cell with up to three different gases.

The large glass cell was then filled with 39 Torr of N₂O. This pressure of N₂O was selected upon reviewing the absorption line data given in the Handbook of Infrared Standards. The data given there was collected at 0.98 Torr and 20 m path length. This gives an optical density of 0.98 Torr times 20 m, or 19.6 Torr-m. Our glass cell was only 0.505 m in length. In order to achieve the same optical density of 19.6 Torr-m and thereby obtain spectra similar to that in the Handbook, the pressure needed was calculated to be 38.8 Torr.

The small cell (Laser Analytics model LOA-005) was similarly evacuated and filled with a pressure of 122.5 Torr N₂O in order to obtain an optical density of 19.6 Torr-m.
Figure 14. Plumbing Network Used to Evacuate the Calibration Cells
The N$_2$O absorption line closest to the measured N$_2$ line was selected as an absolute wavenumber reference point. This, together with the etalon conversion factor enabled an absolute wavenumber scale to be affixed to the N$_2$ scans in place of the abscissa values of laser current.

The particular N$_2$O line was fitted using a non-linear least squares method (see Chapter VII) to locate the line center, i.e., to determine the laser current value that corresponded to the line center. The P(49) line of N$_2$O, located at 2418.64988 ± 0.00010 cm$^{-1}$, was used for the S(10) data, while the P(28)F line of N$_2$O, located at 2433.4738 ± 0.0002 cm$^{-1}$, was used for the S(12) data. The P(49) line belongs to the 12$^D_0$ - 00$^D_0$ band while the P(28)F belongs to the 13$^P_0$ - 01$^P_0$ band according to the notation $v_1$,$v_2$,$v_3$. The symmetrical stretch, bending, and asymmetrical stretch modes correspond to $v_1$, $v_2$, and $v_3$, respectively, with $\ell$ denoting the angular momentum.

IV.5 Beam Expander

A 2.5X beam expander was added to the system to decrease the divergence of the laser beam before it reached the 5 m-focal-length gold mirror as shown in figure 11. The gold mirror was positioned to focus the beam as the beam passed the front surface of the single White cell mirror. If the divergence were too large, the beam, once it reached the opposite end of the White cell would have expanded too much and overfilled the mirror, resulting in a significant loss in signal.

An assortment of lenses were first scanned on a Perkin-Elmer model 1760 Fourier transform spectrometer. One lens was glass and the rest were CaF$_2$. A representative plot of transmission versus wavenumber is given in figure 15 for one of the CaF$_2$ lenses, which does not transmit beyond (to
Figure 15. Representative Plot of Transmission Versus Wavenumber for a CaF$_2$ Lens
wavenumbers smaller than 1000 cm$^{-1}$.

Two lenses were selected after measuring their focal lengths with a collimated light source filtered to emit green light at 0.55 μm. The effective focal lengths of the two lenses at 4.1 μm were 77.330 mm for a 38.14 mm diameter lens, and 195.123 mm for a 50.8 mm diameter lens. The ratio of these effective focal lengths is 2.52. If these lenses are properly positioned, they will expand the beam by this factor.

These lenses were mounted in Daedal mounts for 50.8 mm diameter optics. An adapter was used for the smaller lens. The mount for the smaller lens was then attached to a translation stage, which in turn was attached to a small aluminum plate. This plate was attached at right angles to a thicker aluminum plate, which was also used for mounting the larger lens mount. These mounting procedures were necessary to keep the lenses at the same height yet allowing the small lens to be translated with respect to the larger lens. The distance between the lenses was adjusted initially to the sum of the focal lengths.

The optimal spacing between the lenses was determined to be 24.75 cm by minimizing the far field pattern using the following procedure. Referring to figure 11, the last flat mirror before the White cell was removed and the beam allowed to come to a focus at a distance of 5 m from the gold spherical mirror. In this position, was placed a liquid-N$_2$-cooled InSb detector. An aperture was made for the detector by drilling a 0.0145 inch diameter hole in a thin piece of brass shim stock. This aperture was held to the detector window ring with double-sided tape. The beam waist was sampled by translating the detector up and down and left and right. Small adjustments were made to the beam expander spacing
and the beam waist again measured. This iterative process continued until the beam waist was a minimum of 5.26 mm in the vertical direction, and 5.49 mm in the horizontal direction.

IV.6 Analysis of the N$_2$ Gas Sample

The N$_2$ gas used for this study was rated as 99.998% pure N$_2$ gas obtained from Wince's Welding in Newark, Ohio. The typical analysis of this gas indicated the presence of 5 ppm minimum O$_2$, and 3 ppm H$_2$O.

After all the N$_2$ data was collected, a Varian leak detector was connected with tubing to a valve port in the middle of the 22 m White cell. A 'T' connection was made in this tubing path and connected to a clean stainless steel gas vessel, also via a valve. This plumbing network was evacuated overnight with the valve to the White cell closed. Twice during this period a heat gun was used to heat the gas vessel to aid in the removal of water vapor. The valve to the leak detector was then closed, and the White cell valve opened. The last set of N$_2$ data was collected at ambient pressure ($\approx$1 atm), so the gas vessel was now at that pressure.

This gas sample was taken to the Campus Chemical Instrument Center at Ohio State University and analyzed on a Balzers QME 112 Quadrupole Mass Spectrometer. An average of five scans was taken for a background with a source pressure of $1 \times 10^{-7}$ mbar. An average of five scans was taken of the gas sample with a source pressure of $3 \times 10^{-8}$ mbar. This resulted in the N$_2$, O$_2$, and N concentrations being off scale. The sensitivity was reduced by a factor of 100 and the gas sample was again analyzed. This scan is labelled first sample in Table 8 and indicated that 72.47% was N$_2$, 17.94% was N, 3.99% was H$_2$O, and 1.91% was O$_2$. A second set of five scans was
TABLE 8

MASS SPECTROMETER ANALYSIS OF N₂ GAS SAMPLE

<table>
<thead>
<tr>
<th>m/e</th>
<th>TOTAL %</th>
<th>SPECIES</th>
<th>m/e</th>
<th>TOTAL %</th>
<th>SPECIES</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.27</td>
<td>0.40</td>
<td>H</td>
<td>1.22</td>
<td>0.14</td>
<td>H</td>
</tr>
<tr>
<td>1.98</td>
<td>0.60</td>
<td>H₂</td>
<td>2.04</td>
<td>0.27</td>
<td>H₂</td>
</tr>
<tr>
<td>14.08</td>
<td>17.94</td>
<td>N</td>
<td>6.94</td>
<td>0.19</td>
<td></td>
</tr>
<tr>
<td>16.06</td>
<td>0.99</td>
<td>O</td>
<td>14.08</td>
<td>17.93</td>
<td>N</td>
</tr>
<tr>
<td>17.15</td>
<td>1.17</td>
<td>OH</td>
<td>16.00</td>
<td>0.92</td>
<td>O</td>
</tr>
<tr>
<td>18.11</td>
<td>3.99</td>
<td>H₂O</td>
<td>17.05</td>
<td>0.55</td>
<td>OH</td>
</tr>
<tr>
<td>28.15</td>
<td>72.47</td>
<td>N₁⁵N₁⁵N</td>
<td>18.07</td>
<td>2.11</td>
<td>H₂O</td>
</tr>
<tr>
<td>29.15</td>
<td>0.50</td>
<td>¹⁴N₁⁵N</td>
<td>19.91</td>
<td>0.09</td>
<td>Nê</td>
</tr>
<tr>
<td>32.15</td>
<td>1.91</td>
<td>O₂</td>
<td>28.15</td>
<td>74.99</td>
<td>N</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>29.15</td>
<td>0.55</td>
<td>¹⁴N₁⁵N</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>32.15</td>
<td>2.22</td>
<td>O₂</td>
</tr>
</tbody>
</table>

Taken for a source pressure of 4x10⁻⁶ mbar and averaged together. These data are labelled second sample in Table 8, with the predominant composition being 74.99% N₂, 17.93% N, 2.11% H₂O, and 2.22% O₂. This mass spectrometer could not detect masses greater than 32, such as 44 for CO₂.

Other analysis techniques were investigated because the mass spectrometer analyses were inconsistent with the N₂ gas specifications. The stainless steel gas vessel used to collect the mass spectrometer sample was cleaned with acetone. This cleaning procedure may have left impurities behind, even though the cell was heated several times during the evacuation process. The previous history of this gas vessel was not known.

Furthermore, the maximum vapor pressure of water vapor at 20°C is 17.54 Torr, which corresponds to a H₂O concentration of 2.31%. Since it was not raining in the laboratory (a concentration of 2.31% equates to 100% relative humidity), a more likely concentration would be 0.92% to 1.38% (40% to 60% relative humidity). Regardless, there are no H₂O ab-
sorption lines in the vicinity of the S(10) or S(12) lines of N₂.

Additional analyses were done on samples of gas taken directly from the N₂ gas cylinder, and from the White cell using a MIRAN 1A infrared spectrometer, courtesy of the Owens/Corning Technical Center, Granville, Ohio. Comparisons were made to Airco Industrial Gases "zero-grade" nitrogen, which normally contains, in addition to N₂, 35 ppm Ar, 2 ppm H₂, 10 ppm Ne, 1 ppm O₂, 0.5 ppm CO and CO₂, 0.5 ppm total hydrocarbons (as CH₄), and 3 ppm H₂O. The MIRAN spectrometer was purged with "zero-grade" N₂ and then scanned prior to performing tests on the gas samples.

The first scan was obtained with the N₂ flowing from the gas cylinder through 10 feet of Polyflo® tubing. After 10 minutes of purging a scan was taken over the spectral range from 2.5 to 14.5 μm for a path length of 21.75 m. The spectrum obtained was compared to that taken for the "zero-grade" N₂ and was found to be essentially the same. Both gases contained CO₂ and water vapor at low levels.

The MIRAN spectrometer was then connected to the White cell and the MIRAN was purged for 3-4 minutes with the White cell gas without opening the White cell to the atmosphere. A temperature probe was then removed from one end of the White cell (11 meters away from where the MIRAN was connected) and the MIRAN was purged for two additional minutes. A scan was taken over the same spectral region and path length as before and compared to the trace of the "zero-grade" N₂. This scan showed that both the CO₂ and water vapor levels in the White cell were somewhat higher than in the cylinder N₂. The transmission near the 4.3 μm band of CO₂ was 48% for the White cell and 50% for the "zero-grade" N₂. The transmission due to water vapor in the 6.1 μm region was 7% less for the White cell sample.
(transmission for the "zero-grade" N₂ in this region was 56%). Using equation (51) and the impurity specifications for "zero-grade" N₂, the combined concentration of CO and CO₂ in the White cell sample was at most 0.529 ppm, and the water vapor concentration was at most 3.69 ppm.

The majority of the data was taken at elevated pressures immediately after the White cell had been evacuated and so were unaffected by impurities not already in the N₂ gas cylinder. The one atmosphere data were taken next, at the conclusion of which two leaks were discovered in one end of the White cell. This means that laboratory air containing CO₂ and H₂O could have diffused into the cell during the three-day period of data collection when the pressure was at one atmosphere.

Certain CO₂ lines may interfere with the measurement of the line width of N₂. In the case of the S(10) line of N₂, the P(43) line of CO₂ is the closest at 2418.5803 cm⁻¹. In the case of the S(12) line of N₂, the P(28) line of CO₂ is at 2433.6465 cm⁻¹. The S(10) line was expected to be at 2418.6526 cm⁻¹, which is 0.0723 cm⁻¹ away from the P(43) line of CO₂. Since a resolution of 0.0015 cm⁻¹ was used, the presence of a CO₂ line would have appeared as a separate absorption feature in the scans. No other absorption features were observed, and the resulting transmission versus wavenumber plots did not indicate an asymmetry on the side nearest the CO₂ line. Similarly, no other absorption features or asymmetry were observed in the S(12) scans, in which case the P(28) line of CO₂ was expected to be 0.0571 cm⁻¹ away.
CHAPTER V
COMPUTER HARDWARE AND SOFTWARE

V.1 MINC DECLAB-23 Computer System at OSU

The MINC computer is a Digital Equipment Corporation (DEC) PDP-11/23 processor with 128 kilobytes of metal oxide semiconductor (MOS) memory. It came equipped with two DEC RLO2 10-MByte hard disk drives with removable disk cartridges, a DEC RXO2 floppy disk system containing two disk drives, a DEC LA36 DECWriter printer/terminal, and a DEC VT100 video terminal. Aside from these standard computer peripherals, the MINC also has real-time input/output modules, in particular the MNCAD analog-to-digital (A/D) converter, the MNCAA digital-to-analog (D/A) converter, the MNCDI digital input module, the MNCDO digital output module, and the MNCAG four-channel preamplifier.

Other equipment obtained with the MINC or present in the lab included a Tektronix 4014 terminal, a Tektronix 4630 hard copy unit, a Houston Instruments plotter, and a Kennedy 9000 9-track tape drive with a Kennedy 9217 Formatter.

The tape drive could not be used with the MINC without a tape controller. Most tape controllers are also designed to format tapes. Three companies were identified that sell appropriate tape controllers with formatting capabilities. These are Western Peripheral, Emulex, and Dilog. Magnetic tape is an excellent storage media for collecting a great deal of data, or for making back-up copies of the more expensive RLO2 disk
packs. There is the need to transfer data between laboratories and that transfer medium is often magnetic tape.

The MINC used the RT-11 operating system, and had FORTRAN IV as the standard scientific programming language. A program was developed, entitled DATA.FOR, to collect data from the two lock-in amplifiers to be used in the experiment, to input the changes in position of the echelle via the position sensor circuit, to control the motion of the echelle, to control the current sweep on the laser control module, to coadd scans, to provide a quick plot of the data, and to store the data for future analysis. The object files MNCSNG.OBJ, SYSLIB.OBJ, and FORLIB.OBJ are needed to produce an executable program from DATA.FOR.

The software to produce quality plots and to analyze the data was not integrated into DATA.FOR due to the move of the experiment to Denison University. The laboratory at Denison University utilized a Hewlett-Packard computer system which did not support software written in Fortran. The subroutine PLOTDATA in DATA.FOR was to be replaced with the program CRTPLT.FOR which had been previously developed by the author.

The plotting routine CRTPLT.FOR (Cathode Ray Tube PLoTting routine) uses the Tektronix package PLOT10 to produce professional graphs with a 'best fit' curve and the corresponding value of the integrated area under that curve. CRTPLT will accept input from magnetic tape, digitizing tablet, terminal keyboard, or punched cards and was originally configured to run on an Electronics Associates, Incorporated (EAI) model 640 digital computer. It was planned to add the ability to accept input from disk. This program, after having the data, will plot, apply a polynomial regression fit, and integrate up to 99 curves on the same graph on the
regression fit, and integrate up to 99 curves on the same graph on the Tektronix 4014 terminal. A copy of this plot can be made on the Tektronix 4630 hard copy unit. Linear, semi-logarithmic, or logarithmic plots can be made with CRTPLT.FOR.

This program obviously needs PLOT10.OBJ in addition to SYSLIB.OBJ and FORLIB.OBJ to become executable. It also needs ADEP10.OBJ, which is a short assembly program driver for the Tektronix 4014 terminal.

The source code for the assembly driver, ADEP10.MAC, was not completely debugged. This driver was previously written in EAI assembly code for a Tektronix 4013 terminal and needed to be rewritten in DEC assembly for a Tektronix 4014 terminal. The experiment was moved to Denison before this driver routine could be tested sufficiently. An alternative to ADEP10.MAC would be some combination of routines such as TKCLER.FOR, TKGRPH.FOR, TKOPEN.FOR, TKCLOSE.FOR, TKPLOT.FOR, and TPLOT.FOR which are resident on one of the RLO2 disk packs.

A copy of a detailed operator's manual for CRTPLT.FOR with examples of inputs and outputs was added to the documentation of the MINC DECLAB-23 computer system.

V.2 Link to IRCC via KERMIT

An RS232C interface was installed between the office in room 186 and room 12, where the laboratory is situated, i.e., Smith Lab, Ohio State University. A Micom Local Network model Instamux 470 multiplexer in room 186 allows communication to IRCC or to the Physics Department VAX computer. The other end of the link at room 12 was adapted to enable connection to any of the four channels of the DLV11-J asynchronous serial line unit (SLU) interface of the MINC DECLAB 23 computer system. Each
channel can be configured for nine different baud rates ranging from 150 to 38,400 bits/second. Currently channels SLU 0, SLU 1, and SLU 2 are configured at 9600, 1200, and 300 baud, respectively. These channels are also referred to as serial ports. The fourth channel is labelled "console" and is dedicated to the system terminal.

With a physical link in place to IRCC, the MINC DECLAB-23 computer system can communicate with IRCC if it has the proper software. A RLO2 disk pack was taken to the DEC20 computer system in Hitchcock Hall and all the source code for KERMIT-11 was copied onto it. With this code are several text files which document all aspects of the use of KERMIT. Some of these text files have been printed and are kept with the MINC system. The source code has to be assembled using the Macro-11 assembler program, and then linked before it can be used.

The KERMIT file transfer protocol will allow the MINC to effect error-free file transfer with other computer systems over asynchronous lines. The first implementations would be to communicate with IRCC, e.g., to access magnetic tape data files, or with the Physics Department VAX computer system. Both the MINC and the other system with which it is communicating need to have KERMIT running to effect file transfers.

V.3 Hewlett-Packard 9816 Computer System at Denison University

The computer system used by Denison University with the 22 m White cell consisted of a Hewlett-Packard (HP) 9816 computer, a HP 9134XV hard disk drive, a HP 9121D dual 3.5-inch disk drive, a HP 82905B printer, a HP 3456A digital voltmeter, and a HP 3852A multiprogrammer. The interconnections were shown in figure 14. This computer system is programmed using HP Basic 3.0 and a program had previously been developed.
which controlled the motion of a large grating spectrograph, collected data from the digital voltmeter and a lock-in amplifier, and plotted and stored the data. This program is actually a collection of programs: AUTOST (Auto Start Program), MAC (Multi-Application Controller Program), DACSETUP (Initial Experiment Set-Up Program for the DAC, Data Acquisition and Control System), SYSMAC (Experiment Controller), and DUMPER (program to print raw data). Several other programs were written to complement the ones mentioned above, but were not used to collect N₂ data.

The HP 3852A multiprogrammer was brought on-line to control the current sweep function of the diode laser. Into slot 4 of this multiprogrammer was installed a HP 44727A digital-to-analog (D/A) converter. A multiconductor cable was assembled to connect the D/A converter to the external input BNC of the SP5820 laser control module, to deliver program-directed voltages to the SP5820, and to remotely sense the voltage at the laser control module.

A positive voltage of 10 volts will cause the laser control module to sweep 200 mA. The D/A converter can deliver up to 10 volts with minimum increments of 2.5 mV (corresponding to 0.05 mA). The settling time for the converter is 75 ms, but because the voltages were incremented in small amounts during a scan, the multiprogrammer was directed to allow only 14 ms to the converter before continuing.

In order to collect N₂ data, the collection of programs mentioned above had to be modified to control the current sweep on the laser control module using the HP 3852A multiprogrammer and HP 44727A digital to analog converter, to read the current on the laser control module using the HP 3456A digital voltmeter, and to collect data from a second lock-in
amplifier. The existing software for collecting data from a lock-in amplifier had to be enhanced to prevent the computer from being 'hung', i.e., ceasing to operate, when data was solicited from the lock-in amplifier.

The original programs were left intact. Copies of MAC, DACSETUP, and SYSMAC were made and called MC1, DACSTP2, and SYSMC1. These copies were extensively modified, attempting to preserve the same functions the original programs performed. Listings of MC1, DACSTP2, and SYSMC1 are contained in Appendix A.

In order to use the modified software, the normal start-up procedure for the HP 9816 is interrupted after entering the date and time by holding the shift key down and pressing RESET. The next steps are to type LOAD "DACSTP2:HP913X,703", or simply LOAD "DACSTP2", and to press the RUN key.
CHAPTER VI
DATA COLLECTION PROCEDURES

VI.1 Locating the Spectral Region of Interest

The grating was set to coincide with the spectral region of interest using the calibration described in Chapter IV. This provided a coarse selection of a portion of the electromagnetic spectrum. The slits were left open at 2000 (2 mm). Prior to locating the specific narrow spectral range about a N$_2$ absorption line (a range of 1 cm$^{-1}$), the tuning rate of the laser was determined. The etalon was placed in the beam against the mechanical stops. The output of the detector was viewed on an oscilloscope with the trigger coming from the reference BNC on the laser control module (LCM). The modulation was switched to positive sawtooth (ramp), and the frequency was set to approximately 1 kHz. Full-scale (totally clockwise) on the amplitude dial corresponded to a sweep of 200 mA, which for the diode laser S/N 8020-12 was 2.6 cm$^{-1}$. In order to see a few N$_2$O calibration lines, a sweep of 20 to 30 mA would be sufficient. So the etalon was scanned with a sweep of 20 to 30 mA. The temperature was initially set to 39°K as recommended by Laser Analytics. The current was set to a value at which energy was detected. Diode laser S/N 8020-12 had changed its characteristics with use and required more than the specified 536 mA for normal operation. For the selected amplitude, current, and temperature, a fringe pattern due to the etalon was visible on the scope. No chopper was on or blocking the beam at this point. Having chosen a
fiducial mark on the grid of the scope, the number of fringes that went by was noted as the current was increased. This number divided by the change in current gave the tuning rate in fringes per mA. The fringe spacing for the etalon was approximately 0.048 cm⁻¹. Converting the fringes to wavenumbers yielded the tuning rate in cm⁻¹/ mA.

The narrow spectral range of interest was established by viewing the output of the detector on an oscilloscope with the laser beam passing through the N₂O calibration cell after having removed the etalon from the beam. Again a fiducial mark on the grid of the scope was chosen, and the current was adjusted to align a N₂O absorption line with the mark. This value of the current was recorded. The current was increased or decreased to move the N₂O spectrum across the scope. The current was recorded each time an absorption feature became aligned with the fiducial mark. The currents were converted to wavenumbers using the tuning rate. The relative strengths of the lines were noted also. The resulting pattern of lines was then compared to the spectra of N₂O as given in the Handbook of Infrared Standards. In fact prior to searching for the spectral range with the laser, the appropriate pages were photocopied from this handbook, the spectra cut out with scissors, and the pieces taped together to make one continuous spectrum. Looking at this spectral map and comparing it with the spectrum seen on the scope was often sufficient to locate the spectral region. Small adjustments, in an iterative fashion, on both the current and the laser temperature were required to move to the desired spectral region.

Plots of the three spectral regions of interest are contained in figures 16, 18, and 20 and the corresponding etalon scans are given in
figures 17, 19, and 21 for the \( S(8) \), \( S(10) \), and \( S(12) \) lines, respectively.

VI.2 Detection via Second Derivative Spectroscopy

For second derivative spectroscopy, the modulation was switched to the symmetrical triangular waveform. The amplitude was adjusted to a value of 11.1 mA. This amplitude should be approximately 1.2 times the full-width-half-maximum (FWHM). The FWHM of a quadrupole \( N_2 \) line was thought at the time to be about 0.12 cm\(^{-1}\). The amplitude then was calculated to be 0.144 cm\(^{-1}\) and converted to milliamps using the tuning rate of 0.0129 cm\(^{-1}\)/mA. The tuning rate is relatively constant for a given laser mode.

The current was adjusted to be centered on a \( N_2O \) line known to be close to the \( N_2 \) line of interest. The time base on the oscilloscope was changed to display about four or five triangular wave cycles. Each of these cycles had superimposed on them the same portion of the \( N_2O \) spectrum. The amplitude was further adjusted (decreased) until each cycle appeared symmetrical, much like a sine wave.

Using an EG&G Princeton Applied Research (PAR) 5209 lock-in amplifier set to a frequency of 2f and using the reference out BNC on the LCM as the reference for the lock-in, the signal was maximized by adjusting the gain and phase. The gain was increased because the second derivative signal is weaker than that for straight absorption. Additional increases in signal were obtained by fine adjusting the amplitude on the LCM while viewing the signal on the scope.

The current was decreased to a value of half the desired scan, e.g., 20 mA, and the current sweep control on the LCM was turned on. The
Figure 16. N₂O Scan, S(8) Spectral Region

Figure 17. Etalon Scan for the S(8) Region
Figure 18. \( \text{N}_2\text{O Scan, } S(10) \text{ Spectral Region} \)

Figure 19. Etalon Scan for the \( S(10) \text{ Region} \)
Figure 20. $\text{N}_2\text{O}$ Scan, $S(12)$ Spectral Region

Figure 21. Etalon Scan for the $S(12)$ Region
changes in signal were recorded on an Omega 585 two-channel strip chart recorder. Asymmetrical traces will be observed if the lock-in time constant is too long. The rate of current sweep depends on the steepness of the line. For a broad line a fast rate should be used (1 mA/s or faster), while for a large strong line a slower rate should be used (0.1 mA/s). The scale on the LCM is marked $10^{-4}$ for 0.1 mA/s, $10^{-3}$ for 1 mA/s, etc.

Second derivative chart recorder traces for the detection of the $S(8)$, $S(10)$, and $S(12)$ quadrupole lines of N$_2$ are presented in figures 22, 23, and 24, respectively.

VI.3 Calibration Scans

At the beginning of each set of 20 scans to obtain N$_2$ data at a fixed pressure and temperature, two calibration scans were taken. For one of these scans, the large N$_2$O cell was inserted in the beam (see Chapter IV.4), and for the other, the etalon was inserted into the beam. Figures 16 through 21 are examples of these calibration scans. The etalon scan provides a relative wavenumber scale for the x-axis, while the N$_2$O scan provides absolute wavenumber values corresponding to the locations of the absorption lines.

In addition, a small N$_2$O cell (see Chapter IV.4 and figure 11) was situated to receive a small percentage of the beam from a beamsplitter. A separate detector and lock-in amplifier collected this reference data on every scan simultaneous with the collection of data for the White cell.

VI.4 Straight Absorption Scans

After detecting the presence of a N$_2$ line via second derivative spectroscopy, the modulation and the current sweep on the LCM were turned
Figure 22. Second Derivative Detection of the S(8) Line of $N_2$
Figure 23. Second Derivative Detection of the S(10) Line of N₂
Figure 24. Second Derivative Detection of the S(12) Line of \(N_2\)
off. The PAR 5209 lock-in amplifier was reset back to 1f, the gain was
decreased, and the phase readjusted for direct absorption measurements.
A PAR model 192 chopper running at 469 Hz provided the modulation.
Generally the same spectral region that was scanned in second derivative
mode was scanned in direct absorption mode. Some refinements were made
to center the scan on the $N_2$ line.

The LCM was made to current sweep under computer control and the
digital data stored for each scan. The temperature and pressure in the
White cell were recorded at ten minute intervals with the aid of a HP
3467A data logger. A total of 20 scans was taken for each pressure.

VI.5 Summary of Measurement Conditions

All three lines were detected using second derivative spectroscopy.
Only the S(10) and S(12) lines were characterized in direct absorption.
The temperature was kept constant at ambient for all scans. Twenty scans
were taken of the S(10) line at each of three White cell pressures: 734,
837, and 730 Torr. The last set of scans was taken a week after the first
to confirm the reproducibility of the data. Twenty scans were taken of
the S(12) line at each of five pressures: 837, 880, 950, 732, and 729
Torr. The redundant set of scans at 729 Torr was taken to check system
operation because the signal level was lower than usual.
CHAPTER VII
DATA ANALYSIS

VII.1 Pre-processing of Data

All of the data were recorded onto single-sided 3.5-inch floppy disks in Hewlett-Packard binary. After all the scans were completed, back-up copies of the data were made onto 5.25-inch floppy disks using a Hewlett-Packard 9836 computer system equipped with an auxiliary disk drive for 3.5-inch floppies (HP 9122D).

In order to facilitate the data analysis on a different computer system, the same HP 9836 computer was used to read in the binary data and convert it to ASCII. The OVERLAY section of SYSMAC was modified to perform this function. A listing of this modified code is given in Appendix B. The ASCII produced by a Hewlett-Packard computer is in Logical Interchange Format (LIF). Even though ASCII is a universal method of interchanging data, an additional conversion was necessary to make the ASCII files legible to an IBM-compatible personal computer (PC) such as the Zenith Supersport 286 laptop computer which was used to process the data.

A program entitled PCLIF.EXE, written by Innovative Software Systems, version 2.50, 1986, was used to read the LIF ASCII files and convert them to PC ASCII. An auxiliary 5.25-inch floppy disk drive was used with the Zenith Supersport 286 computer to read the LIF ASCII files.

The data acquisition program, SYSMAC, used at Denison University...
stored the data in three arrays: the laser current (x values), the signal observed after the laser beam passed through the White cell (y values), and the reference signal after the laser beam passed through a calibration cell (r values). The OVERLAY section of SYSMAC, after modification to store the data in ASCII, stored the data in the sequence $x_1, y_1, r_1, x_2, y_2, r_2,$ etc. instead of storing the entire $x$ array, then the entire $y$ array, followed by the entire $r$ array. Therefore a sorting program was needed. A short program was written in GWBASIC to read in the data, after it had been converted to PC ASCII, and to group all the $x$ values together, the $y$ values together, and the $r$ values together.

VII.2 Shifts in Laser Current (Wavenumber)

The sorted data for each of the 222 scans were imported into Lotus 1-2-3 (123), a spreadsheet program to facilitate the mathematical manipulation of the data and to view the data graphically. A business graphics program, Freelance Plus, version 3.0, also a Lotus product, was used in conjunction with 123 to graphically determine the required shifts in laser current (i.e., cm$^{-1}$) for each scan prior to the coaddition of scans.

Using 123, a composite file was constructed of all twenty $N_2O$ reference scans, which were taken with the small $N_2O$ cell, in a given observation set. Typical digitized $N_2O$ scans were given in figures 18 and 20. Portions of this composite file were imported into Freelance by using the Datalinks feature.

Using the Axis Scaling feature, values were selected for the minimum and maximum of the x-axis, and for the major and minor grid intervals for the x-axis so that the region around the absorption line was enlarged on the screen. In the case of the $S(12)$ line, one of the reference $N_2O$ lines
was the P(33) line. For the minimum and maximum x-axis (laser current in amperes) values, 0.683 and 0.690 were entered, respectively, while 0.001 and 0.0002 were entered for the major and minor x-axis grid intervals, respectively. The selection of minimum and maximum x-axis values ensured that only the P(33) region filled the screen, and the choice of grid intervals allowed the rapid determination of the required shifts in laser current. The use of the grid intervals will be further discussed below.

The Zenith 286 laptop computer has a graphics display of 640 x 400 pixels. The field of interest, 0.683 to 0.690 ampere, was then divided into 640 pixels, each representing $1.09 \times 10^{-6}$ ampere, although the raw data was collected at increments of $1.0 \times 10^{-4}$ ampere. In this example, each data point was separated by approximately nine pixels, and 70 data points were displayed.

One of the reference scans out of a set of 20 taken at a fixed pressure was chosen to be fixed in x (laser current). A N₂O scan which occurred at the beginning of the set of twenty scans was usually chosen as the reference scan with respect to laser current because it followed the etalon scan. Data from this scan were imported as the $x_1$ and $y_1$ values. Data from each of the remaining scans in an observation set (twenty scans) were always imported as the $x_2$ and $y_2$ values. So two curves were displayed with the objective of moving the $(x_2,y_2)$ curve in x until it was coincident with the $(x_1,y_1)$ curve.

Using the menu above the plotted data, a short vertical line segment was added to the plot, usually at the location of a grid mark on the x-axis, below the absorption minima. This line was always one pixel wide regardless of the scale used. Next the $(x_2,y_2)$ curve and the line segment
were selected and the Split feature was used to enable the selected items to be moved while everything else remained stationary. It was important to note over which x-axis grid line the added line segment was drawn. This line segment was now either to the right or left of this position after moving the \((x_2, y_2)\) curve to make it coincident with the \((x_1, y_1)\) curve. The amount of shift in laser current needed to make the curves coincident was the difference between the before and after positions of the added line segment.

In order to calculate this difference in positions, Freelance was instructed to zoom into that portion of the plot containing the before and after positions of the added line segment, as well as the corresponding portions of the labelled x-axis. The cursor was activated and moved from the before to the after positions of the added line segment, while counting the number of times the right (or left) arrow was pressed to move the cursor (which corresponded to the number of pixels). This number divided by the number of pixels needed to advance to the next grid interval, multiplied by the grid spacing, gave the desired shift in laser current. An upper bound on the uncertainty in these graphically-determined shifts would be one-half the increment between data points, or \(5 \times 10^{-8}\) ampere. The uncertainty is somewhat less than this because the absorption features were smooth, continuous curves despite the fact that the data was collected every 0.0001 ampere and despite the fact that Freelance connected the data points with straight line segments. Furthermore, differences in the overlap of two \(\text{N}_2\text{O}\) curves could easily be discerned with changes as small as \(5 \times 10^{-8}\) ampere for the \(S(12)\) data at 837 Torr. Using the appropriate etalon tuning rate from Table 7, an uncer-
tainty of $5 \times 10^{-6}$ ampere corresponds to $7 \times 10^{-5}$ cm$^{-1}$.

The laser current values of the $(x_2, y_2)$ curve were numerically shifted using 123. A new column was created in the 123 file of each scan which equaled the original current plus (or minus) the shift value. Another column was created which produced interpolated values of the White cell signal voltage (i.e., $N_2$ data) which could be used with the original laser current values.

**VII.3 Curvature Comparisons**

After shifting the data horizontally in laser current, the twenty $N_2$ curves in a given observation set were examined for changes in curvature. The same procedure was used to manipulate the $(x_2, y_2)$ curve in the $y$-direction as was used in the $x$-direction to determine the laser current shifts. The $(x_2, y_2)$ curve was moved in the $y$-direction until it was coincident with the $(x_1, y_1)$ curve. In this case, the $(x_1, y_1)$ curve was not necessarily the reference. No numerical information was extracted during this process. The curves were merely compared visually. If the $N_2$ curves had the same curvature over most of the spectral region, and, in particular, in the vicinity of the $N_2$ line, then a note was made that these curves could be coadded together. The curvature changed enough between scans to warrant grouping and coadding only $N_2$ curves of similar curvature. A set of 20 curves (for a specific $N_2$ line at a specific pressure) was typically divided into five or more groups.

**VII.4 Background Fits**

The ideal data analysis sequence would be to coadd twenty scans of data in a given set, fit a polynomial to the background excluding the absorption feature, ratio the coadded data to the background, then fit
the resulting absorption line using a non-linear least squares routine. The non-linear least squares method is discussed in the next section.

As mentioned previously, the full set of twenty scans could not be coadded directly but were coadded within smaller groups. An example of a single \( \text{N}_2 \) scan and of ten \( \text{N}_2 \) scans averaged together are given in figures 25 and 26, respectively, for the S(10) line at 734 Torr. A polynomial was fitted to each coadded composite curve using least squares and excluding the region containing the \( \text{N}_2 \) line. Figure 27 shows a computed background fit superimposed onto the averaged data of figure 26. Figure 28 is a plot of transmission versus laser current obtained by ratioing the background and data plots of figure 27. If as a result of grouping and coadding, a set of 20 curves were reduced to five curves, then five background fits were performed. The five background curves were each divided by the corresponding data curve to obtain five plots of transmission versus laser current. These five transmission curves were then coadded (averaged) together by weighting each curve by the number of scans that were originally averaged together to obtain that curve. This final plot was then fitted with a straight line (excluding the \( \text{N}_2 \) line) which corresponded to 100% transmission. After ratioing the data and the straight line, the \( \text{N}_2 \) line was fitted using a non-linear least squares routine to obtain the line center, full-width-at-half-maximum (FWHM), and equivalent width.

VII.5 Non-Linear Least Squares Fits (Marquardt's Method)

The resulting absorption lines were fit using Marquardt's method as coded in the program SPECTRA and used at Denison University on a VAX 11/785 computer system. The program SPECTRA also performed the background
Figure 25. Single N$_2$ Scan

Figure 26. Ten N$_2$ Scans Averaged Together
Figure 27. Background Fit

Figure 28. Transmission vs. Laser Current
fits to data as described in the previous section. Marquardt's method is briefly summarized below.

The Marquardt algorithm can be summarized as an iterative process with five basic steps:

1) Evaluate the residual error, RE. If it is small enough, then stop. The residual error is given by

\[ \text{RE} = \sum_i [f(x_i; q^0) - d_i]^2 \]  \hspace{1cm} (102)

where \( d_i \) is a data point, \( x_i \) is the \( i^{th} \) set of independent variables, and \( f \) is the function that is intended to represent the data. The set \( q^0 \) consists of estimates of parameters in \( f \) that are to be determined by the fit. At this point in the analysis the raw or coadded data had been ratioed to the least squares polynomial background fit. The resulting curve of transmission versus laser current (e.g. figure 28) was the absorption feature emanating from a flat baseline. The background fit used for the baseline was a straight line and the function \( f \), which was used to describe the absorption feature, was a Gaussian. The Gaussian fit produced significantly smaller residuals than did a Lorentzian fit.

2) Evaluate the response of the residual error to changes in the \( q \) as a Taylor series through quadratic terms. The Taylor series is

\[ \text{RE}(q) = \text{RE}(q^0) + \sum_a \frac{\partial \text{RE}}{\partial q_a} (q_a - q^0_a) + \frac{1}{2} \sum_{a,n} \frac{\partial^2 \text{RE}}{\partial q_a \partial q_n} (q_a - q^0_a)(q_n - q^0_n) \]  \hspace{1cm} (103)

where

\[ \frac{\partial \text{RE}}{\partial q_a} = \sum_i 2[f(x_i; q^0) - d_i] \frac{\partial f}{\partial q_a} \]  \hspace{1cm} (104)
The second term in equation (105) is dropped as an approximation. If \( B \) is the vector of first derivatives of \( RE \), \( A \) is the matrix of second derivatives, and \( \Delta \) is the vector of the displacements \( dq \) in each parameter, then the residual error can be written as

\[
RE(q) = RE(q^0) + \Delta^T B + \Delta^T A \Delta
\]

or

\[
RE(q) = RE(q^0) + \Delta^T(B + A\Delta)
\]

If \( q^0 \) corresponds to a minimum in \( RE(q) \), the coefficient of \( \Delta \) will be zero.

3) Choose \( \Delta \) so that

\[
B + A\Delta = 0, \text{ or } \Delta = -A^{-1}B
\]

and consider \( q^0 + \Delta = q \) to be a better description of the least-squares optimized set of parameters.

4) If needed, revise the step length \( \Delta \) defined in the "steepest descents" direction, i.e., alter \( q^0 \) by a \( \Delta \) which produces the most drastic decrease in \( RE \). The matrix \( A \) may become singular in which case it cannot be inverted. In the Marquardt method, \( A \) is replaced by \( A + \lambda I \). The parameter \( \lambda \) is chosen so that \( A + \lambda I \) is non-singular, i.e., \( \det(A+\lambda I) \neq 0 \), and so that the step \( \Delta(\lambda) = (A + \lambda I)^{-1}B \) is guaranteed to decrease the residual error. The original point \( q^0 \) has a steepest descents direction defined locally. A very short step will lead to a lower residual error, but a long step may not. The step length is short if \( \lambda \) is large, and could be long if \( \lambda \approx 0 \). The parameter \( \lambda \) provides a way to pick through a steep, rapidly changing contour.
5) Return to step 1.

The Marquardt method is a compromise between the methods of Gauss-Newton and steepest descent. As $\lambda \to 0$, the method approaches Gauss-Newton. As $\lambda \to \infty$, the method approaches steepest descent. Marquardt's method is equivalent to performing a series of ridge regressions and is useful when the parameter estimates are highly correlated or the objective function is not well approximated by a quadratic.

After all the fits to the data were done, the x-axis was converted from laser current in amperes to wavenumber units using the calibration data given in Chapter IV. As mentioned in that chapter, the $P(49)$ or $P(28)F$ line of $N_2O$ was fitted using the program SPECTRA to obtain its line center in terms of laser current. The scan taken of the small $N_2O$ cell, which had been used as the reference for shifting the other 19 scans in a set, was used as input to SPECTRA. The $P(49)$ line served as an absolute calibration point for the $S(10)$ data, while the $P(28)F$ line was used for the $S(12)$ data. For these lines as well as the final $N_2$ transmission curves, a cursor was used to identify to SPECTRA that region of the plot which contained the absorption line. A background fit was then performed of the data excluding the absorption region. Third, fourth, or fifth order polynomials were used and SPECTRA immediately displayed the data plot with the background fit superimposed on it. The polynomial fit provided a continuous curve which followed the data up to the absorption line, passed over the absorption line as if building a bridge, and continued following the data beyond the absorption line. If the particular order of fit was acceptable to the user (i.e., had the minimum variance), then SPECTRA ratioed the data to the background. At this
point, a non-linear least squares fit to the ratioed data was performed and displayed with the ratioed data. The line center and equivalent width, along with coefficients of the background fit and the \((x,y)\) positions of the non-linear fit in the region of the absorption feature, were obtained from three output files.

The uncertainty of the background fit depended on the user's choice, via the cursor, of the region of the plot to be excluded (the absorption feature), as well as on the order of fit selected. The output file containing the background fit coefficients also provided the standard deviation of the fit selected as well as of all lower order fits. Obviously the standard deviation could only be calculated for that region of the data plot which did not contain the absorption line.

Given the line center of the appropriate \(\text{N}_2\text{O}\) line in units of amperes, this value was compared to the column of x-axis values in the 123 file of the reference \(\text{N}_2\) scan. In most cases this laser current value fell between two laser current values associated with the x-axis of the \(\text{N}_2\) data. Using the accepted wavenumber position for the \(\text{N}_2\text{O}\) line, a linear interpolation was done to compute the wavenumber position of the nearest x-axis laser current. From this computed wavenumber position and the tuning rate of the etalon, the x-axis values were converted from amperes to cm\(^{-1}\). The uncertainties in this procedure depended on the accuracy of the \(\text{N}_2\text{O}\) line position (in amperes) as determined by SPECTRA, as given in terms of wavenumber units as obtained from handbooks, and on the accuracy of the etalon tuning rate.

The full-width at half-maximum (FWHM) values were determined prior to converting the x-axis to wavenumber units. The non-linear least squares
fit using a Gaussian had three adjustable parameters: the height, the line center, and the FWHM. The FWHM values, in units of amperes, were converted to \(\text{cm}^{-1}\) using the appropriate etalon tuning rate.

### VII.6 Integrated Absorption and Quadrupole Moment Derivatives

In the weak line limit, which was applicable here, the equivalent width, \(W\), approaches the integrated absorption, \(S\), times the optical density, \(\text{n}_x\), i.e., \(W = S \times \text{n}_x\). The equivalent width was obtained from the non-linear least squares fit by integrating between the fit and baseline. Simpson's rule was used to approximate the area. The integrated absorption was calculated from the data by dividing the equivalent width by the optical density. The uncertainty in \(S\) will then depend on the uncertainties in the equivalent width, the concentration \((\text{n})\), and the path length \((x)\).

The derivative of the quadrupole moment was found using equation (71) after a value was obtained for the integrated absorption, \(S_{\nu}(T)\). The factor \(8\pi^5/15hc\) was computed to be \(8.216 \times 10^{17}/\text{erg cm}\). The lower state energies, \(E\), used for the \(S(10)\) and \(S(12)\) lines were 218.783 and 310.233 cm\(^{-1}\), and they were converted to ergs by multiplying by \(hc\). Using the values or formulas given in Chapter II for \(g_J\), \(2J+1\), \(Z(T)\), and the square of the Clebsch-Gordan coefficients, equation (71) simplified to

\[
S_{\nu}(T) = (3.152 \times 10^{16}/\text{erg cm}) \nu^3 |\langle 0|Q|1\rangle|^2
\]

(109) for the \(S(10)\) line. The factor 3.152 was replaced with 2.374 for the \(S(12)\) line. Using the procedure mentioned above, the integrated absorption was in units of \(\text{cm}^2\text{atm}^{-1}\). Multiplying this by \(1.3626 T \times 10^{-22}\) converted it to units of \(\text{cm/molecule}\). The square root of the expectation value of \(Q\) was found to be \(3.188 \times 10^{-10}\) cm times \(\delta Q/\delta r\). Solving equation...
(109) for $\partial Q/\partial r$, the units were esu cm. One debye (D) is $1 \times 10^{-18}$ esu cm or $3.335641 \times 10^{-18}$ C m. The derivative of $Q$ was then converted to debyes and then to units of $e_0$ ($e_0 = 2.542$ D).
CHAPTER VIII
DISCUSSION OF RESULTS AND CONCLUSIONS

VIII.1 Motivation
In the space shuttle data\textsuperscript{11}, the S(8), S(10), and S(12) lines were observed without interference at a resolution of 0.002 cm\textsuperscript{-1}. It has been suggested that these lines be used as calibration points with respect to the determination of tangent height and line of sight column density, provided some means could be devised to calibrate these lines in the laboratory.

VIII.2 Experimental Design
A diode laser is a source of radiation which can be tuned over an absorption line using an ultimate resolution of 0.0003 cm\textsuperscript{-1}. With this in mind, an experiment was planned to include a diode laser for the S(8) region of the spectrum and a White cell adjusted to a 5 km path length. The S(8) line was initially selected because it has the greatest intensity of the three N\textsubscript{2} lines mentioned above. The path length was chosen to simulate the path lengths used by the Jungfraujoch facility\textsuperscript{18}, by ATMOS on the space shuttle\textsuperscript{10,11}, and by Camy-Peyret et al.\textsuperscript{9} at Kitt Peak.

A diode laser was ordered for the S(8) region prior to the common use of molecular beam epitaxy to fabricate it. The diode was received nearly a year after it was ordered because the production of a diode which operated in the correct spectral region and which lased was accomplished by trial-and-error. It was found however that the output of the laser
was insufficient to characterize the S(8) line through 5 km of path. Instead the diode was observed to emit sufficient energy in the S(10) and S(12) regions of the spectrum, which were subsequently characterized as a function of pressure.

A considerable amount of development was required to achieve the 5 km path in the laboratory. The problem was basically one of aligning an emitting surface of 10 μm by 10 μm with a detector that was 5 km away. This alignment was hampered by the constant vibration induced by the piston in the cold head, and the finite size of the image (5 mm x 5 mm) on the White cell mirror, which in turn limited the maximum achievable path length to 1.67 km. An innovation that facilitated the achievement of the 5 km path length was the use of three retroreflector assemblies (see figures 6 and 10) which allowed the beam to traverse the White cell three times, each time travelling 1.67 km.

VIII.3 Basic Results

The specific purpose of the experiment was to obtain measurements of the half-widths and equivalent widths of the lines through direct absorption scans, but in the process, evidence was also observed for pressure-induced collisional narrowing. The S(10) quadrupole absorption line of N₂ was characterized at 730, 734, and 837 Torr and plots of transmission versus wavenumber are given in figures 29, 30, and 31, respectively. The non-linear least squares fits to these absorption lines are shown in these figures as dotted lines. Similarly, the S(12) quadrupole absorption line of N₂ was measured at 729, 732, 837, 880, and 950 Torr. The corresponding figures for these conditions are 32 through 36, respectively. All
Figure 29. \( S(10) \) Quadrupole Absorption Line at 730 Torr
Figure 30. $S(10)$ Quadrupole Absorption Line at 734 Torr
Figure 31. S(10) Quadrupole Absorption Line at 837 Torr
Figure 32. S(12) Quadrupole Absorption Line at 729 Torr
Figure 33. S(12) Quadrupole Absorption Line at 732 Torr
Figure 34. S(12) Quadrupole Absorption Line at 837 Torr
Figure 35. $S(12)$ Quadrupole Absorption Line at 880 Torr
Figure 36. S(12) Quadrupole Absorption Line at 950 Torr
data were collected for a path length of 5.016 km and a temperature of 297°K.

Values for the line center, equivalent width, full-width-at-half-maximum (FWHM), and percent extinction and percent absorption at line center are given in Table 9. Following the procedures given in Chapter VII for the calculation of line center positions and FWHM values, and using the appropriate error formulas as derived from equation (100) for each mathematical operation, the uncertainties in the last digits of the data are given in Table 9 in parentheses to the right of the value. The line center and two values of percent extinction for the S(8) line of N₂ are also given in Table 9. These values were obtained from the second harmonic detection traces of figure 22.

Integrated absorption, Sᵥ(T), and the derivative of the quadrupole moment, ∂Q/∂r, together with uncertainties, are given in Table 10. As was mentioned in Chapter VII, the uncertainty in the integrated absorption will depend upon the errors in the equivalent width, the path length, and the pressure. The error in the derivative of the quadrupole moment will depend on the error in the integrated absorption as well as on the error in all the other factors in equation (71).

The HITRAN database⁶⁶ was consulted for the currently accepted line centers of the two N₂ lines that were studied here. The line centers of the S(10), and S(12) lines at 760 Torr are given by HITRAN to be located at 2418.6548, and 2433.5893 cm⁻¹, respectively. Comparing line centers measured at similar pressures, the S(10) line at 734 Torr differs from the HITRAN value at 760 Torr by 0.0033 cm⁻¹, while the S(12) line at 732 Torr
TABLE 9

SUMMARY OF BASIC RESULTS

<table>
<thead>
<tr>
<th>Line</th>
<th>Pressure (Torr)</th>
<th>Line Center (cm⁻¹)</th>
<th>Equiv. Width (10⁻⁶ cm⁻¹)</th>
<th>FWHM (cm⁻¹)</th>
<th>% Ext.</th>
<th>% Abs.</th>
</tr>
</thead>
<tbody>
<tr>
<td>S(8)</td>
<td>730</td>
<td>2403.514(8)</td>
<td></td>
<td></td>
<td>2.76(38), P(10) ref.</td>
<td>1.68(26), P(65) ref.</td>
</tr>
<tr>
<td></td>
<td>734</td>
<td>2418.6457(4)</td>
<td>1.913(2)</td>
<td>0.0733(9)</td>
<td>1.671(3)</td>
<td>1.668(3)</td>
</tr>
<tr>
<td></td>
<td>837</td>
<td>2418.6581(2)</td>
<td>1.813(2)</td>
<td>0.0741(4)</td>
<td>1.566(7)</td>
<td>1.563(7)</td>
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<td>887</td>
<td>2418.6552(3)</td>
<td>1.661(2)</td>
<td>0.0698(2)</td>
<td>1.522(21)</td>
<td>1.519(21)</td>
</tr>
<tr>
<td>S(10)</td>
<td>730</td>
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<td>1.913(2)</td>
<td>0.0733(9)</td>
<td>1.671(3)</td>
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<td>1.813(2)</td>
<td>0.0741(4)</td>
<td>1.566(7)</td>
<td>1.563(7)</td>
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<td>2418.6552(3)</td>
<td>1.661(2)</td>
<td>0.0698(2)</td>
<td>1.522(21)</td>
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<td>1.661(2)</td>
<td>0.0698(2)</td>
<td>1.522(21)</td>
<td>1.519(21)</td>
</tr>
<tr>
<td>S(12)</td>
<td>729</td>
<td>2433.5609(5)</td>
<td>2.063(2)</td>
<td>0.0905(10)</td>
<td>1.458(22)</td>
<td>1.456(22)</td>
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<td>732</td>
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<td>3.006(3)</td>
<td>0.0965(12)</td>
<td>1.979(20)</td>
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<td>0.853(1)</td>
<td>0.0628(7)</td>
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<td>0.865(14)</td>
</tr>
<tr>
<td></td>
<td>880</td>
<td>2433.6062(4)</td>
<td>1.376(1)</td>
<td>0.0731(7)</td>
<td>1.203(23)</td>
<td>1.200(23)</td>
</tr>
<tr>
<td></td>
<td>950</td>
<td>2433.5937(4)</td>
<td>1.729(2)</td>
<td>0.0834(7)</td>
<td>1.326(4)</td>
<td>1.322(4)</td>
</tr>
</tbody>
</table>

TABLE 10

QUADRUPOLE MOMENT DERIVATIVES

<table>
<thead>
<tr>
<th>Line</th>
<th>Pressure (Torr)</th>
<th>Sν(297°K)/10⁻⁹ (cm⁻² atm⁻¹)</th>
<th>Sν/10⁻²⁸ (cm/molecule)</th>
<th>∂Q/∂r (ea₀)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S(10)</td>
<td>730</td>
<td>3.971(5)</td>
<td>1.607(2)</td>
<td>0.742(21)</td>
</tr>
<tr>
<td></td>
<td>734</td>
<td>3.742(4)</td>
<td>1.514(2)</td>
<td>0.721(21)</td>
</tr>
<tr>
<td></td>
<td>837</td>
<td>3.007(4)</td>
<td>1.217(2)</td>
<td>0.646(19)</td>
</tr>
<tr>
<td>S(12)</td>
<td>729</td>
<td>4.288(4)</td>
<td>1.735(2)</td>
<td>0.881(25)</td>
</tr>
<tr>
<td></td>
<td>732</td>
<td>6.222(6)</td>
<td>2.518(3)</td>
<td>1.061(31)</td>
</tr>
<tr>
<td></td>
<td>837</td>
<td>1.544(2)</td>
<td>0.625(1)</td>
<td>0.528(15)</td>
</tr>
<tr>
<td></td>
<td>880</td>
<td>2.369(2)</td>
<td>0.959(1)</td>
<td>0.654(19)</td>
</tr>
<tr>
<td></td>
<td>950</td>
<td>2.758(3)</td>
<td>1.116(1)</td>
<td>0.706(20)</td>
</tr>
</tbody>
</table>
differs from the HITRAN value at 760 Torr by 0.0014 cm⁻¹. Considering the resolution used to obtain the N₂ data which is currently in HITRAN (0.009 cm⁻¹ at best), the agreement is very good.

The average of $\delta Q/\delta r$ at pressures near one atmosphere was found to be $(0.732 \pm 0.015) \text{ cm}^{-1}$ for the S(10) line and $(0.971 \pm 0.127) \text{ cm}^{-1}$ for the S(12) line. Previous studies show agreement with the S(12) result but not the S(10) result. Camy-Peyret et al.⁹ gave values of 0.95 cm⁻¹ and 0.97 cm⁻¹ for the S(12) and S(10) lines at an atmosphere of pressure, respectively, while Reuter et al.¹² gave values of 0.965 cm⁻¹ and 0.909 cm⁻¹ for the S(12) and S(10) lines at 605 Torr, respectively. The lack of agreement for the S(10) line may be due to the lower resolution used by these previous authors, which in turn will give a less reliable estimate of the equivalent width. The equivalent width is one of the main factors used to determine $\delta Q/\delta r$. Another contributing factor may be due to the fact that Reuter et al. used a Lorentzian profile to fit these weak lines. This choice of line profile was found to be inappropriate for the data depicted in figures 29 through 36. This point is further discussed in the next section.

VIII.4 Collisional Narrowing

Some of the full-widths observed by Reuter et al.¹² were 0.0572 and 0.1808 for the S(10) line and 0.0618 and 0.1254 cm⁻¹ for the S(12) line at 605 and 1580 Torr, respectively. Figure 37 is a plot of the S(12) FWHM values from Table 9 and from Reuter et al. The straight line in figure 37 is a least squares fit to the three S(12) data points (249, 605, and 1580 Torr) of Reuter et al. The data obtained by Reuter et al. is roughly consistent with the data in the present work, but a direct comparison is
Figure 37. Full-Width-Half-Maximum versus Pressure.
difficult to make considering the resolution used in each case. Reuter et al. used resolutions of 0.025 and 0.050 cm\(^{-1}\) for the 605 Torr and 1580 Torr data, respectively. The data given in Table 9 were taken with a resolution of 0.0015 cm\(^{-1}\). A least squares linear fit to the full-width values in Table 9 of the S(12) line as a function of pressure (837, 880, 950 Torr), including zero full-width at zero Torr, gave a slope of 8.3 \times 10^{-5} \text{ cm}^{-1}/\text{Torr} (or 0.06308 cm\(^{-1}\)/atm) and an intercept of -6.9 \times 10^{-4} \text{ cm}^{-1}. Using this fit, the FWHM at 732 Torr would have been 0.0601 cm\(^{-1}\), which is comparable to the value that Reuter et al. obtained at 605 Torr.

If the data (twenty scans) taken at 732 Torr had only been observed once, then it might be viewed with doubt. However, data at that pressure (729 Torr) were taken again the next day and essentially the same FWHM was observed. These data suggest that collisional narrowing of the line is occurring, with a minimum near 837 Torr, using the data of Table 9. The occurrence of collisional narrowing has been observed in quadrupole lines of hydrogen\(^{57}\) and in vibrational-rotational transitions in HCl:Ar mixtures\(^{58}\).

The collisional narrowing of lines is not a process that is unique to hydrogen. It may occur in any gas spectra, but is not usually observed because pressure broadening is generally dominant before the effect sets in. The Dicke\(^{69}\) profile, which assumes that the quadrupole line shape is Lorentzian with a half-width that varies inversely as the pressure, was found to be an invalid approximation for computing collision-narrowed profiles of hydrogen quadrupole lines at visible and near infrared wavelengths in any hydrogen atmosphere\(^{57}\). The line shape that did fit the hydrogen data was the Galatry\(^{60}\) profile, which is more like a Gaussian
function than a Lorentzian. The Galatry profile is composed of a sum of Lorentzian functions. At high pressures (> 2 atm), the series is dominated by the first Lorentzian expression so that the line has a Lorentz shape\(^7\). For the small range of relatively low pressures over which the \( \text{N}_2 \) lines were observed, the Lorentzian line shape was not found to be appropriate.
APPENDIX A

DATA ACQUISITION SOFTWARE FOR THE HEWLETT-PACKARD 9816
DACSETUP
Initial Experiment Set-Up Program for the
DAC
Data Acquisition and Control system
by Kip Shaffer
6/88
Last Revised 4/8/89 by Paul P. Balog

DIM ES$(35)(80)
OUTPUT 2:" K":
PRINT " SET-UP Program"
PRINT "Enter the title of the experiment (include"
PRINT "monochromator dial/slit setting/laser temp.)"
LINPUT ES$(1)
PRINT "List by code separated by commas the devices to be used in the expe-
rintment."
PRINT ",1.1 Stepper-motor-controlled grating"
PRINT "2.1 HP 44727A DAC (to diode laser control module)"
PRINT "3.1 HP 3495A DVM"
PRINT "4.1 PAR 5209 Lock-in Amplifier"
PRINT "4.2 PAR 5207 Lock-in Amplifier"
LINPUT ES$(2)
ES$(3)="1232323" ! Scan Sequence List (Currently Disabled)
ES$(4)="1 2 3" ! Plot Switch List, by Scan Step Type
ES$(5)="1 2 3" ! Co-Add Switch List
LINPUT "What is the abscissa display device code (e.g., 2.1)?",ES$(12)
IF ES$(12)="1.1" THEN GOTO 237
IF ES$(12)<"2.1" THEN GOTO 151
LINPUT "Enter Starting LCM Current (-2 A to 2 A).",ES$(6)
E6=VAL(ES$(6))
IF E6<-2.0 OR E6>2.0 THEN GOTO 154
ES$(7)=E6
LINPUT "Enter Current Sweep in milliamps (0 to 200 mA).",ES$(7)
E7=VAL(ES$(7))
IF E7<0 OR E7>200 THEN GOTO 158
NOTS=E7/.05 ! Minimum increment on DAC(2.5 mV) corresponds to .05 mA
PRINT "The maximum number of data points per scan is",NOTS
LINPUT "Enter step in milliamps in format of XXX.X",ES$(9)
E9=VAL(ES$(9))
IF E9<0 OR E9>200 THEN GOTO 174
ES$(7)=E6-E7/1000
ES$(9)=-E9/1000
ES$(7)=-ES$(7)
CASE ELSE
END SELECT
PRINT "The actual number of data points per scan will be",E9m
LINPUT "Enter Lock-in Amplifier Time Constant in Seconds.",ESa$
E8=E9m*(VAL(ESa$)*3)
Me8=E8/60
PRINT "Each scan will take",E8," seconds, or".INT(ME8)," minutes and",FRAC
T(ME8).GO," seconds."
INPUT "Is this acceptable (Y or N)?",X$
SELECT X$
  CASE "Y", "y"
  GOTO 206
CASE "N", "n"
CASE ELSE
  GOTO 158
END SELECT
PRINT "Enter + for fast(14 ms), or - for standard(75 ms) DAC turnaround",E$(11)
IF E$(11)<"+" A N D  E$(11)<"-" THEN GOTO 245
END SELECT
  CASE E$(17)
  CASE "N", "n"
  CASE ELSE
  GOTO 287
END SELECT
LINPUT "Enter number of scans.",ES(21)
CASE "Y", "y"
CASE ELSE
  GOTO 338
END SELECT
  CASE E$(22)
  CASE "N", "n"
  CASE ELSE
  GOTO 336
END SELECT
  CASE E$(23)
  CASE E$(24)
  CASE "X" 1  Co-Add Function Specifier
  CASE "Y" 1  Run Time Status Line
LINPUT "Operator's name",OPNAM$
Dds$="HPB290X,700,1"
INPUT "Default File Spec (four letters max)(HeNe)>",DFS$
INPUT "Scan ID number (four digits max) (100) ",Sid
X$=VAL$(Sid)
ASSIGN @Save TO "DACDEF"
OUTPUT @Save;E$(*)
OUTPUT @Save;OPNAM$
OUTPUT @Save;DFS$
OUTPUT @Save;X$
ASSIGN @Save TO *
DISP "DACDEF now saved..."
MAC

Multi Application Controller Program
1987

by Kip Shaffer

MASS STORAGE IS "HP913X,703"

DIM Residency(10)

Ms$(1)="HP8290X,700,0"
Ms$(2)="HP8290X,700,1"
Ms$(3)="HP83902,702"
Ms$(4)="HP913X,703"

Dk$(1)="0"
Dk$(2)="A"
Dk$(3)="C"

Dk$(4)="C"

Start=1

COM Goio,Dev_control

COM /Disk/ Dk,Dk$(1:4){1}.Ms$(1:4){14}

COM /Disk/ Dk(1:100){80}.Dk(1:100){80}.Cat_count(1:2).Disk_change(1:100,1 :2).Comment$(1:100,1:2){56}

GINIT

PLOTTER IS 3,"INTERNAL"

CLEAR

OUTPUT 2;" K";

GRAPHICS ON

PEN 1

VIEWPORT 0,130.15,130

FRAME

ON KEY 9 LABEL "Exit" GOTO 410

ON KEY 5 LABEL "Menu" GOTO Menu

ON KEY 1 LABEL "Change Disk" GOTO 340

ON KEY 7 LABEL "Data Box" GOTO 382

ON KEY 6 LABEL D$ GOTO 301

IF Start=1 THEN Menu

Wait:

PRINT TABXY(3.1):DATES(TIMEDATE);

PRINT TABXY(68.1):TIMES(TIMEDATE MOD 86400);

GOTO Wait

Menu:

Menu Line=1

M=1

PRINT TABXY(10.7+Menu_line);"--";

ON KNOB .1 GOTO Knob

ON KBD GOTO Kbd

Start=0

GOTO 160

Knob:

PRINT TABXY(10.7+M1);" ":

Menu_line=Menu_line+KNDBX/5

IF Menu_line<1 THEN Menu_line=1

IF Menu_line>4 THEN Menu_line=4

M1=INT(Menu_line)

PRINT TABXY(10.7+M1);"--";

GOTO Wait

Kbd: A=S+KBD$
280  OFF KNOB
282  SELECT A$ 
283  CASE "E"
284  GOTO Menu_choice
286  CASE "1"
287  GOTO Disku
288  CASE "2"
289  GOTO Setup
290  CASE "3"
291  GOTO Experiment
292  CASE "4"
293  GOTO Databox
294  CASE ELSE
295  BEEP
296  PRINT TABXY(1,2);"<";NUM(A$);">"
297  GOTO Wait
298  END SELECT
299  Menu_choice: ON M1 GOTO Disku,Setup,Experiment,Databox
300  Catalog: GRAPHICS OFF
301  OFF KNOB
302  OFF KBD
303  OUTPUT 2;" K"
304  OFF KEY 7
305  CAT
306  PRINT TABXY(10);CHR$(129);"Use wheel to scroll display.";CHR$(128)
307  GOTO 300
308  Changedisk: Dk=Dk+1=A*(Dk=4)
309  D$="Catalog <"&D$&">"
310  MASS STORAGE IS Ms$$(Dk)
311  GOTO 200
312  Disku: IF Resident(1)>1 THEN 375
313  LOADSUB ALL FROM "DISCMAC:703"
314  Resident(1)=1
315  CALL Diskutil
316  GOTO Menu
317  Setup:
318  OUTPUT 2;" K"
319  GCLEAR
320  LOAD "DACSTP2";
321  Databox: IF Resident(3)>1 THEN 395
322  LOADSUB ALL FROM "DACBUG:703"
323  Resident(3)=1 ! Flag routines are resident
324  CALL Daq
325  GOTO Menu
326  Experiment:
327  OUTPUT 2;" K"
328  LOAD "SYSMCI:HP913,703";
329  !-------------------------------------------------------------------------------------------------------------------------end
330  GCLEAR
331  GRAPHICS OFF
332  OUTPUT 2;" K"
333  END
334  !-------------------------------------------------------------------------------------------------------------------------sub routines
SYSMAC

Experiment Controller

1987-1988 by (Kip) John D. Shaffer

Last Revised by Paul P. Balog on 4/2/89

------------------------------------------------------------------------------------------------------------

<table>
<thead>
<tr>
<th>COM / Parameters/ D(4096,6), Indev_parms$(18,8)[20], Outdev_parms$(18,5,3)[20], Devname$[10][20], Exp_control$[23][80], Numparm</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>COM / Param2/ Opnam$[80], Dds$(20), Dfs$[4], Sid, Auto$[10][40]</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>COM / Extra/ Numadded, D_element, Maxmin(10,2)</th>
</tr>
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</table>

<table>
<thead>
<tr>
<th>Numparm=25</th>
</tr>
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<table>
<thead>
<tr>
<th>Autoscan=0 ! first autoscan command</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Num_channels=0</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Tone=1 ! default is tone ON</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Tune=1 ! default is Tune Mode ON</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>DIM Plib(10)</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>DIM Choice$(18)[80], Indata$(18,1), Control_params$(10)[10], Ovl(4096,6), Bcd_data$(20), Desc$(18)[40]</th>
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</table>

<table>
<thead>
<tr>
<th>DIM $(180), QS$(80), TS$(80), BS$(80), VS$(80), A$(20)</th>
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<table>
<thead>
<tr>
<th>COM Gpio, Dev_control</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Gpio=12 ! GPIO Port</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Seq_no=1 ! Scan Sequence No.</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Demo=0 ! Do initial Graphics.</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Sline=10 ! Screen Line.</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Overlay=0 ! No overlay files specified</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>New_screen: GCLEAR ! Draw Screen Section  ********************************************************************</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>OUTPUT 2;&quot; K&quot;;</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>GINIT</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>GRAPHICS ON</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>VIEWPORT 0,97,45,130</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Xmin=0</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Xmax=4096</th>
</tr>
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</table>

<table>
<thead>
<tr>
<th>Ymin=0</th>
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</thead>
</table>

<table>
<thead>
<tr>
<th>Ymax=0</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>PEN 1</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>FRAME</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>DATA 61,3, &quot;Scan Sequence:&quot; , &quot;Use arrows &lt;-&gt; to change sequence step&quot;</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>DATA 61,5, &quot;Plot Switch:&quot; , &quot;Press 1, 2, or 3 to toggle&quot;</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>DATA 61,7, &quot;Co-adding:&quot; , &quot;Hit &lt;Space&gt; to toggle&quot;</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>DATA 61,8, &quot;Co-added:&quot; , &quot;Press control-C to clear co-addition data&quot;</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>DATA 63,11, &quot;Start&quot;: &quot;Press &lt;Space&gt; to enter new Starting value&quot;</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>DATA 63,12, &quot;Finish&quot;: &quot;Press &lt;Space&gt; to enter new Finishing value&quot;</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>DATA 63,13, &quot;Current&quot;: &quot;Press &lt;Space&gt; to enter new Current value&quot;</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>DATA 63,14, &quot;Step&quot;: &quot;Press &lt;Space&gt; to enter new Step size value&quot;</th>
</tr>
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<table>
<thead>
<tr>
<th>DATA 63,15, &quot;Delay&quot;: &quot;Press &lt;Space&gt; to enter new Delay time (sec.)&quot;</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>DATA 61,16, &quot;Experiment&quot;: &quot;Press &lt;C&gt; to Start Scan, &lt;C&gt; to Clear Scan, Up/D own to modify&quot;</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>PRINT TABXY(61,1):CHR$(129);&quot; Experiment Control&quot;;CHR$(128)</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>PRINT TABXY(61,10):&quot; Abcissa Info. &quot;</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>RESTORE</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>FOR I=1 TO 10</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>READ X,Y,AS,Q$</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>NEXT I ! End Draw Screen Section  ********************************************************************</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>ReadDefaults!: Recall defaults, define devices, etc.</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>! MASS STORAGE IS &quot; : HP8290X, 700, 0&quot;</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>! MASS STORAGE IS &quot; : MEMORY, 0, 1&quot;</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>MASS STORAGE IS &quot; : HP913X, 703&quot;</th>
</tr>
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</table>

<table>
<thead>
<tr>
<th>IF Opnam$=&quot; THEN</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>ASSIGN @Recall TO &quot; DACDEF: HP913X, 703&quot;</th>
</tr>
</thead>
</table>
ASSIGN @Recall TO "DACDEF:HP8290X,700.0"
ENTER @Recall;Exp_control$(*)
ENTER @Recall;Dps$
ENTER @Recall;Dfs$
ENTER @Recall;X$
Sid=VAL(X$)
ASSIGN @Recall TO  
END IF
CALL Unpack(Num_elements, Pack$(*) , Exp_control$(2))
Num_channels=Num_elements
L-1
Devnames:!  ----Read in device names
TS=Exp_control$(2)
R_loop_2: X=POS(T$,""") IF X<>0 THEN
READ Devname$(L)
TS=TS(X+1)
L=L+1
GOTO R_loop_2
END IF
Screen_draw: ! Fill in blanks to right of graph ------------------------
GOSUB Draw_graph
PRINT TABXY(1.15);CHR$(132):"Window Values: Y-axis:<Ymin):";VAL$(Ymin)
PRINT TABXY(1.16);CHR$(132):"Ymax):";VAL$(Ymax)
PRINT TABXY(1.17):"**
PRINT TABXY(1.18):"SCAN TITLE IS:":Exp_control$(1)
PRINT TABXY(25.16):"Current Job Name:";Dfs$(1:4);VAL$(Sid)
PRINT TABXY(73.16);CHR$(130):"Stopped":CHR$(128)
PRINT TABXY(62+Seq_no,11);CHR$(129);Exp_control$(3)[Seq_no]+1
PRINT TABXY(72.7);" 
IF POS(Exp_control$(5),Exp_control$(3)[Seq_no])<>0 THEN PRINT "Yes"
ELSE PRINT "No"
END IF
PRINT TABXY(72.8):Numadded
PRINT TABXY(72.9);Numadded
PRINT TABXY(72.11);TS[1:8]
PRINT TABXY(72.12):TS[1:8]
PRINT TABXY(72.13);TS[1:8]
PRINT TABXY(72.14);TS[1:8]
PRINT TABXY(72.15);TS[1:8]
IF Demo=1 THEN
FOR I=1 TO 500
D(I,1)=I=2
D(I,2)=SIN(I/500/.333*PI)*(-50)+50
NEXT I
END IF
GOSUB Tone_toggle
GOSUB Tune_toggle
157 GOSUB Tone_toggle
158 GOSUB Tune_toggle
159 ON KEY 9 LABEL "Exit" GOTO End
160 ON KEY 4 LABEL "Print Data" GOSUB Printdata
161 ON KEY 6 LABEL "Menu" GOTO Menu
162 ON KEY 8 LABEL "Cat Data Disk" GOTO Cat
163 ON KEY 3 LABEL "Overlay File" GOTO Overlay
164 ON KEY 1 LABEL "Printer Dump" GOTO Printer_dump
165 ON KEY 5 LABEL "TEST KEY" GOTO Read_volt
166 IF Expo<>0 THEN GOTO Start_scan
169 Expcontrol: !---------------Modify Experiment Parameters
170 RESTORE
171 FOR I=1 TO Sline
172 READ X,Y,PS,QS
173 NEXT I
174 PRINT TABXY(X,Y);CHR$(129);PS;CHR$(128)
175 DISP QS
176 ON KBD GOTO Edit
177 Wait: GOTO Wait
178 Edit: !------------------------Actual Editing Routines
179 AS=KBD$0
180 OFF KBD
181 SELECT AS
182 CASE "E" "." ":"
183 PRINT TABXY(X,Y);PS
184 Sline=Sline+(Sline<10)+1
185 CASE " "
186 PRINT TABXY(X,Y);PS
187 Sline=Sline+(Sline<1)+10
188 CASE ELSE
189 SELECT Sline
190 CASE 1
191 IF AS=" >" THEN Seq_no=Seq_no+1*(Seq_no<LEN(Exp_control$)<3))
192 IF AS=" <" THEN Seq_no=Seq_no-1*(Seq_no<1)
193 IF POS("123",AS)<0 AND LEN(Exp_control$)<3)<15 THEN
194 T1$=Exp_control$<3>(1,Seq_no-1)
195 T2$=Exp_control$<3>(Seq_no-1)
196 Exp_control$<3>=T1$+T2$
197 Seq_no=Seq_no+1
198 END IF
199 IF AS=" B" AND Seq_no>1 THEN
200 T1$=Exp_control$<3>(1,Seq_no-2)
201 T2$=Exp_control$<3>(Seq_no-1)
202 Exp_control$<3>=T1$+T2$
203 Seq_no=Seq_no-1
204 END IF
205 IF AS=" -" AND LEN(Exp_control$)<3))>1 THEN
206 T1$=Exp_control$<3>(1,Seq_no-1)
207 T2$=Exp_control$<3>(Seq_no+1)
208 Exp_control$<3>=T1$+T2$
209 IF Seq_no<LEN(Exp_control$)<3)) THEN Seq_no=Seq_no-1*(Seq_no
210 END IF
211 GOTO 127
212 CASE 2
213 XS=Exp_control$<4>
214 GOSUB Toggle123
215 Exp_control$<4>=TS
216 GOTO 129
217 CASE 3
218 XS=Exp_control$<5>
IF A$=" " THEN
    A$=Exp_control$(3)(Seq_no;1)
    GOSUB Toggle123
    Exp_control$(5)=I$
    END IF
GOTO 130
CASE 4
    IF A$=CHR$(3) THEN
        FOR I=1 TO 500
            D(I,0)=0
        NEXT I
    END IF
    GOTO 130
CASE 5,6,7,8
    IF A$=" " THEN
        INPUT "Enter new value below":,X
        X=VAL(H$&Exp_control$(6))
        Y=VAL(H$&Exp_control$(7))
        Z=VAL(H$&Exp_control$(9))
        Exp_control$(9)=VALS(ABS(Z)*SGN(Y-X))
        FOR I=1 TO 4
            Outdev_paramS(I,1,1)=Exp_control$(I+5)
        NEXT I
        END IF
CASE 9
    IF A$=" " THEN
        INPUT "Enter new delay between data points",Exp_control$(27)
    END IF
GOTO 145
CASE 10
    IF A$="G" OR A$="g" THEN GOTO Start_scan
    IF A$="c" OR A$="c" THEN
        INPUT "Are you sure? <Y/N>",X$}
        SELECT X$}
            CASE "Y","y"
                D_element=1
                GOTO Screen_draw
            CASE "N","n"
            CASE ELSE
                END IF
        END SELECT
    END IF
    END SELECT
GOTO Expcontrol

Toggle123:
X=0
FOR I=1 TO 3
    X=X+2 I*(POS(X$&VALS(I))<>0)
    NEXT I
    IF POS("123",A$)<0 THEN X=BINEOR(X,2^VAL(A$))
    TS=....
FOR I=1 TO 3
    IF BIT(X,I) THEN
        TS=TS&VALS(I)&" "
    END IF
GOTO Expcontrol
ELSE
  TS=TS&" "
END IF
NEXT I
RETURN

Start_scan: !-----------------------------------------------------------------------------Start Scan
OFF KBD
X=VAL("0"&Auto$(0))
IF X>0 AND Expgo>1 THEN
  Autoscan=Autoscan+1
  IF Autoscan>=Num_channels THEN Autoscan=1
  TS=Auto$(Autoscan)
  DISP "Auto Command:";TS
  SELECT TS[1:5]
  CASE "Set L"
    Exp_control$(6)=TS[12,POS(TS," ")-1]
    Exp_control$(7)=TS[POS(TS," ")+1]
    GOTO 287
  CASE "Set S"
    Exp_control$(9)=TS[10,POS(TS,"units")-1]
    GOTO 287
  CASE "Set D"
    Exp_control$(27)=TS[11,POS(TS,"seconds")-1]
    GOTO 287
  CASE "Scan"
    Exp_control$(20)=TS[6,POS(TS,"times")-1]
    Expgo=1
    GOTO Screen_draw
  CASE "Wait"
    N=VAL(TS[5,POS(TS,"minutes")-1])*60
    WAIT N
    GOTO 287
END SELECT
END IF
Expgo=0
GCLEAR
FRAME
DISP
Start_time$=TIME$(TIMEDATE)
OFF KEY
ON KEY 0 LABEL "Pause Exp." GOTO Pause
! Update name on screen:
PRINT TABXY(1,10);"SCAN TITLE IS:";Exp_control$(1)
PRINT TABXY(25,16);"Current Job Name:";Dfs$[1:4];VAL$(Sid+1);" "
D_element=1
! Clear Max Min's for new data
FOR I=1 TO Num_channels
  Maxmin[I,1]=0
  Maxmin[I,2]=0
NEXT I
! Start at beginning...
Exp_control$(8)=Exp_control$(6)
IF Exp_control$(12)="2.1" THEN GOTO 337
GOSUB Abcissa
GOTO 346
! GOSUB Tune_toggle
OUTPUT 710;"SWRITE 400,2.13"
IF Exp_control$(11)="+" THEN OUTPUT 710;"SWRITE 400,17.00"
IF Exp_control$(11)="-" THEN OUTPUT 710;"SWRITE 400,91.00"
CLEAR 710
151

343  OUTPUT 710; "APPLY DCV 400,0" !INITIALIZE DAC
344  CLEAR 712
345  !Initialize Volt Meter if needed
346  IF FNDev_on$(3,1,Exp_control$2)="Y" THEN
347     FOR I=1 TO 8
348         Choice$(I)=Indev_param$(3,1)
349     NEXT I
350     CALL Dv_init((1),Choice$(*)
351  END IF
352
353  CLEAR 712
354
355  IF FNDev_on$(4,1,Exp_control$2)="Y" THEN
356     FOR I=1 TO 8
357         Choice$(I)=Indev_param$(3,1)
358     NEXT I
359     CALL Lockin_readt1.Choicest"), Indata"))
360  END IF
361
362  !Get data
363  Choice$(0)=Exp_control$(2)
364  FOR I=1 TO 8
365      Choice$(I)=Indev_parm$(1,1)
366  NEXT I
367  CALL Dac_readt1.(Choice$(*).,Indata(*))
368  IF FNDev_on$(3,1,Exp_control$(2))="Y" THEN
369      FOR I=1 TO 8
370          Choice$(I)=Indev_parm$(3,1)
371      NEXT I
372      CALL Lockin_readt1.Choicest"), Indata"))
373  END IF
374
375  Exp_loop:------------------------------------------SCAN
376  From=VAL(Exp_control$(6))
377  To=VAL(Exp_control$(7))
378  Step=VAL(Exp_control$(8))
379  FOR Expl=From TO To STEP Step
380      PRINT TABXY(73,15): "Running"
381      Exp_control$t8)=VAL(Exp$t8)
382      IF Exp_control$(12)="2.1" THEN GOTO 366
383      GOSUB Abcissa ! Stepper-motor-controlled grating
384      GOTO 367
385  END IF
386  GOSUB Dac_lcm ! HP 4472A DAC to diode laser
387  WAIT VAL(Exp_control$(27))
388  Numdev=Num_channels
389
390  !Get data
391  Choice$(0)=Exp_control$(2)
392  FOR I=1 TO 8
393      Choice$(I)=Indev_parm$(1,1)
394  NEXT I
395  CALL Dac_readt1.(Choice$(*).,Indata(*))
396  IF FNDev_on$(3,1,Exp_control$(2))="Y" THEN
397      FOR I=1 TO 8
398          Choice$(I)=Indev_parm$(3,1)
399      NEXT I
400      CALL Lockin_readt1.(Choice$(*).,Indata(*)
401  END IF
402
403  GO TO 367
404
405  IF Tune=1 THEN D0_element, 1)=Expl
406  IF Tune=1 THEN D0_element, 2)=Expl
407  IF Tune=1 THEN D0_element, 3)=Expl
408  IF Tune=1 THEN D0_element, 4)=Expl
409  IF Tune=1 THEN D0_element, 5)=Expl
410  IF Tune=1 THEN D0_element, 6)=Expl
411  IF Tune=1 THEN D0_element, 7)=Expl
412  IF Tune=1 THEN D0_element, 8)=Expl
413
414  366  GOSUB Add_point
415  IF Tune=1 THEN D0_element, 1)=Exp$1
416  IF Tune=1 THEN D0_element, 2)=Exp$2
417  IF Tune=1 THEN D0_element, 3)=Exp$3
418  IF Tune=1 THEN D0_element, 4)=Exp$4
419  IF Tune=1 THEN D0_element, 5)=Exp$5
420  IF Tune=1 THEN D0_element, 6)=Exp$6
421  IF Tune=1 THEN D0_element, 7)=Exp$7
422  IF Tune=1 THEN D0_element, 8)=Exp$8
152

END IF
405 IF D_element > 1 THEN
406 PEN -1
407 PENUP
408 PLOT Y, Ymin
409 PLOT Y, Ymax
410 END IF
411 PEN 1
412 PENUP
413 PLOT Y, Ymin
414 PLOT Y*Step, Ymin
415 PLOT Y*Step, Ymax
416 PLOT Y, Ymax
417 PENUP
418 PLOT Py, Pt
419 PLOT Y, T
420 IF Tone = 1 THEN
421 IF T < Ymax THEN BEEP 5080*T/Ymax, .1
422 BEEP 400, .1
423 END IF
424 PRINT TABXY(16, 17); " ";
425 IF Exp_control$12) <> "2.1" THEN GOTO 431
426 T = T + 1000
427 R = R - 1000
428 PRINT TABXY(20, 17); "Sig."; TABXY(33, 17); "mV"; TABXY(40, 17); "Ref."; R;
429 PLOTXY(51, 17); "mV"
430 GOTO 434
431 PRINT TABXY(16, 17)
432 ! Co add point
433 IF POS(Exp_control$5, Exp_control$3(Seq_no; 1)) > 0 AND Tune = 0 THEN
434 D(D_element, 0) = D(D_element, 0) + D(D_element, FNChan_no(Exp_control$23, Exp_control$2))
435 END IF
436 ! END IF
437 FOR I = 0 TO Num_channels
438 IF D(D_element, I) > Maxmin(I, 1) THEN
439 Maxmin(I, 1) = D(D_element, I)
440 END IF
441 IF D(D_element, I) < Maxmin(I, 2) THEN
442 Maxmin(I, 2) = D(D_element, I)
443 END IF
444 NEXT I
445 ! ready next point
446 PRINT TABXY(72, 13); " ";
447 PRINT TABXY(72, 13); D(D_element, 2)
448 D_element = D_element + 1
449 IF D_element > 4096 THEN Pause
450 NEXT Expl
451 !
452 !
453 !
454 !
455 !
456 Scan_is_done:
457 IF Exp_control$12) <> "2.1" THEN
458 OUTPUT 710; "APPLY D C V 400, 0" ! CLEAR DAC
459 OUTPUT 722; "S 06STG 10 STI" ! CLEAR DVM
460 END IF
461 GOSUB Draw_graph
462 OFF KEY 0
463 Num_scans = Num_scans + 1
465  IF Exp_control$(17) = "Y" THEN GOSUB Savetodisk
466  ! IF Tune = 1 THEN GOTO Screen_draw
468  IF Exp_control$(26) = "Y" THEN
469  ! DISP "Printing Status Line"
470  OUTPUT 701
471  OUTPUT 701: "Scan"; Num_scans; " of ": Exp_control$(20) completed. ":Exp_control$(1)
472  OUTPUT 701;
473  OUTPUT 701; "Start Time: ";: Start_time$;
474  OUTPUT 701; " End Time: ";: End_time$;
475  OUTPUT 701; "Scan Limits "::Xmin; "Xmax"
476  OUTPUT 701; "Operator: "::Opnam$;
477  END IF
478  OUTPUT 701; "";
479  DISP
480  END IF
481  Num_added = Num_added + POS(Exp_control$(5); Exp_control$(3)); Seq_no; 1)
482  Seq_no = Seq_no + POS(Exp_control$(3));
483  IF Num_scans < VAL(Exp_control$(20)) THEN !do another scan...
484  Expgo = 1
485  ELSE
486  END IF
487  Num_scans = 0
488  END IF
489  IF VAL("0" = Auto$(0)) <> 0 THEN Expgo = -1
490  IF Exp_control$(19) = "Y" THEN GOTO Printer_dump
491  GOTO Screen_draw
492  !
493 !
494  !
495  Return: ON KEY 0 LABEL "Resume Exp." GOTO Continue_scan
496  GOTO Screen_draw
497  Continue_scan: !
498  OFF KBD
499  OFF KEY
500  ON KEY 0 LABEL "Pause Exp." GOTO Pause
501  GOTO 362
502  Abcissa: !
503  IF Tune = 1 THEN RETURN
504  FOR I = 1 TO 5
505  Control_param$ (I) = Exp_control$ (I + 5)
506  NEXT I
507  CALL Stepper control(Control_param$)
508  FOR I = 1 TO 5
509  Exp_control$(I + 5) = Control_param$(I)
510  NEXT I
511  RETURN
512  Dac_lcm: !
513  V1 = ABS(Exp_from); 1000/20
514  V2 = SGN(From_to)
515  V1 = V1 * V2
516  PRINT "V DAC-"; V1
517  BS = VAL(V1)
518  AS = "APPLY DCV 400."
519  BS = AS
520  OUTPUT 710; BS
521  RETURN
522  Add_point: !
523  FOR I = 1 TO Numdev
524  DQ_element[I] = Indata(I, 1)
525  IF Exp_control$(12) = "2.1" THEN GOTO 530
IF I=2 THEN D(D_element,2)+D(D_element,2)*.008066

Find maximum and minimum values:
IF D(D_element,1)>Maxmin(I,1) THEN
    Maxmin(I,1)=D(D_element,1)
END IF
IF D(D_element,1)<Maxmin(I,2) THEN
    Maxmin(I,2)=D(D_element,1)
END IF

NEXT I

Print data: !
X-FNChan_no(Exp_control$<12>,Exp_control$<2>)
Y-FNChan_no(Exp_control$<13>,Exp_control$<2>)
R-FNChan_no("4.2",Exp_control$<2>)
FOR I=1 TO D_element STEP 2
    J=I+1
    K=I+2
    OUTPUT 701;D(I,X),D(I,Y),D(I,R),D(J,X),D(J,Y),D(J,R),D(K,X),D(K,Y),D(K,R)
NEXT I
RETURN

Draw graph: !
IF Exp_control$<14>="Y" AND D_element>2 THEN
    Ymax=Maxmin(FNChan_no(Exp_control$<13>,Exp_control$<2>),1)
    Ymin=Maxmin(FNChan_no(Exp_control$<13>,Exp_control$<2>),2)
    Top=Ymax
    Bottom=Ymin
    R=(Ymax-Ymin)*.05
    Ymin=Ymin-R
    Ymax=Ymax+R
END IF

IF Exp_control$<14>="N" OR Ymax=Ymin THEN
    CALL Unpack("N"),Pack$(1),Exp_control$<15>
    Ymin=VAL(Pack$(1))
    Ymax=VAL(Pack$(2))
    Top=Ymax
    Bottom=Ymin
END IF

WINDOW Xmin, Xmax, Ymin, Ymax
GCLEAR
FRAME
PEN 1
LINE TYPE 1
PENUP
MOVE D(1,1),0
X-FNChan_no(Exp_control$<12>,Exp_control$<2>)
Y-FNChan_no(Exp_control$<13>,Exp_control$<2>)
PRINT "X,Y=" X,Y
PAUSE
FOR I=1 TO D_element-1
    Div=1
    IF Numadded>0 THEN Div=Numadded
    IF VAL(Exp_control$<20>)=1 THEN Y=0
    PLOT D(I,X),D(I,Y)/Div
NEXT I

FOR I=1 TO Overlay+1
    X-FNChan_no(Exp_control$<12>,Exp_control$<2>)
    Y-FNChan_no(Exp_control$<13>,Exp_control$<2>)
    MOVE Div(I,1),0
NEXT I
593      PLOT Ov(I,X),Ov(I,Y)
594      NEXT I
595      LINE TYPE 1
596 END IF.
597 AXES (Xmax-Xmin)/20.0,Xmin-INT((Xmax-Xmin)/10),Ymin,2
598 AXES (Xmax-Xmin)/20.0,Xmin-INT((Xmax-Xmin)/10),Ymax,2
599 AXES 0,(Top-Bottom)/20,Xmin,Bottom-INT((Top-Bottom)/10),1,2
600 AXES 0,(Top-Bottom)/20,Xmax,Bottom-INT((Top-Bottom)/10),1,2
601 RETURN
602 Savetodisk:!
603 IF Iy=0
604   Sid=Sid+1
605   T$=Dfs$+VAL$(Sid)\&Dfs$
606 ON ERROR GOTO Disk_error
607 CREATE BDAT T$,D_element+20,Num_channels=8
608 OFF ERROR
609 ASSIGN @Dataout TO T$
610 DISP "Saving Data to ":T$
611 OUTPUT @Dataout:Exp_control$<1)
612 OUTPUT @Dataout:Exp_control$<2)
613 OUTPUT @Dataout:Exp_control$<3)(Seq_no:11&","&VAL$(D_element)
614 OUTPUT @Dataout:DATES(TIMEDATE)&","&TIMES(TIMEDATE)
615 OUTPUT @Dataout:Dname$
616 OUTPUT @Dataout:"=
617 OUTPUT @Dataout:"=
618 OUTPUT @Dataout:"=
619 OUTPUT @Dataout:"=
620 OUTPUT @Dataout:"=
621 IF Exp_control$<12)>"2.1" THEN GOTO 625
622 X=FNChan_no("2.1",Exp_control$<2))
623 Y=FNChan_no("4.1",Exp_control$<2))
624 R=FNChan_no("4.2",Exp_control$<2))
625 FOR I=1 TO D_element
626 IF Exp_control$<12)>"2.1" THEN GOTO 634
627 IF Iy=1 THEN
628 OUTPUT @Dataout;(I,X),D(I,0)/Num_scans,D(I,R)
629 GOTO 632
630 END IF.
631 OUTPUT @Dataout:(I,X),D(I,Y),D(I,R)
632 OUTPUT @Dataout
633 GOTO 63B
634 FOR J=1 TO Num_channels
635 OUTPUT @Dataout:D(I,J);
636 NEXT J
637 OUTPUT @Dataout
638 NEXT I
639 ASSIGN @Dataout TO =
640 DISP
641 IF Iy=1 THEN
642 Dfs$=Dfs$
643 RETURN
644 END IF.
645 IF Exp_control$<22)=>"Y" AND Num_scans+VAL(Exp_control$<20)) THEN
646 Iy=1
647 Dfs$=Dfs$
648 Dfs$=Dfs$&"C"
650 GOTO 604
652 END IF.
653 RETURN
654 Disk_error:!!
655 SELECT ERRN
CASE 54
    DISP 'Ts:"a duplicate file name... Finding next valid name."
    S;S=S+1
    GOTO 605
CASE 64
    DISP "Data disk FULL! Please place blank disk in drive and press <
     CONT>"
    PAUSE
    GOTO 605
CASE 65
    DISP "Disk Write Protected! Please fix and press <CONT>"
    PAUSE
    GOTO 605
CASE 66
    DISP "Disk not initialized! Please try another disk and press <CONT
     >"
    PAUSE
    GOTO 605
CASE ELSE
    DISP "Unknown error:";ERRN
    PAUSE
    END SELECT
    GOTO 605
Printer_dump:
    GOSUB Printer_dump_2
    GOTO New_screen
Printer_dump_2:
    CLEAR
    VIEWPORT 0,65,65,130
    VIEWPORT 0,130,0,130
    OUTPUT 2;" K";
    OFF KEY
    GOSUB Draw_graph
    OUTPUT 701;RPT$("",.67);Ymax
    LOADSUB ALL FROM "DUMPER:HP8290X,700,0"
    CALL Dumper(400,400,""
    CALL Dumper(200,108,"Y-Scale: "&VAL$(Ymin)&": "&VAL$(Ymax))
    Y$="Y-Scale:"&VAL$(Ymin)&": "&VAL$(Ymax)
    OUTPUT 701;Y$
    DELSUB Dumper
    X$="X-Scale:"&VAL$(Xmin)&": "&VAL$(Xmax)
    OUTPUT 701;X$  RPT$("",70-LEN(X$));Ymin
    OUTPUT 701;"Scan Filenam e:";DFS$&VAL$(S;)
    IF Overlay-1 THEN
    OUTPUT 701;"Overlay Filenam e:";OvI$
    END IF
    OUTPUT 701; ""
    RETURN
Menu:!
CALL Window
GOTO Screen_draw
Cat:!
GRAPHICS OFF
OUTPUT 2;" K";
CAT ":HP8290X,700,1"
DISP "Hit <Space> to continue"
ON KBD GOTO Cont
Loop: GOTO Loop
Cont: OFF KBD
OUTPUT 2;" K";
GRAPHICS ON
GOTO New_screen

INPUT "Specify: 'NULL', 'CURRENT', 'SCAN', or a valid Filename",X$
SELECT X$
CASE "NULL";"" ! ANY OVERLAYS ARE CANCELLED.
OVERLAY=0
CASE "CURRENT" ! TURNS BACK ON AN OVERLAY FILE "NULL" TURNED OFF.
OVERLAY=1
CASE "SCAN" ! PUTS CURRENT SCAN INTO OVERLAY ARRAYS.
X=FNChan_no(Exp_control$(12),Exp_control$(2))
Y=FNChan_no(Exp_control$(13),Exp_control$(2))
FOR I=1 TO 4096
Ov(I,1)=D(I,X)
Ov(I,2)=D(I,Y)
NEXT I
Ov$=Dfs$&VAL$(Sid)
Ov(0,0)=0_element-1
OVERLAY=1
CASE ELSE ! RETRIEVES A FILE FROM DISK TO BE OVERLAID.
Ov$=X$
IF Exp_control$(12)="2.1" THEN
Rs=1
CLEAR ! CLEAR GRAPHICS
OUTPUT 2;"K"; ! CLEAR SCREEN
PRINT "Enter R(to divide current scan by overlay file),"
PRINT "or S(to input file as overlay file without ratioing),"
PRINT "or SD(to input file as current scan),"
PRINT "or C(to coadd a series of files),"
PRINT "or T(to divide overlay file by current scan)."
LINPUT Rs
SELECT Rs$
CASE "R","r"
LINPUT "DO YOU WANT TO RATIO TO REF.LOCK-IN? (Y OR N)",X$
SELECT X$
CASE "Y","y"
Rls="Y"
CASE "N","n"
Rls="N"
CASE ELSE
GOTO 752
END SELECT
CASE "S","s"
Rs="S"
CASE "SD","sd"
Rs="SD"
CASE "C","c"
Rs="C"
LINPUT "LAST SCAN TO BE CO-ADDED? (Y OR N)",X$
IF X$="N" THEN GOTO 776
IF X$="Y" THEN GOTO 768
INPUT "ENTER TOTAL # OF SCANS.".Ns
CASE "T","t"
Rs="T"
CASE ELSE
GOTO 743
END SELECT
END IF
ON ERROR GOTO Disk_in_error
ASSIGN @Input TO Ov$&Dfs$
159

843 Tone_toggle:
844 IF Tone=1 THEN
845 Tone=0 ON KEY 2 LABEL "Tone is OFF" GOSUB Tone_toggle
847 ELSE
848 Tone=1 ON KEY 2 LABEL "Tone is ON" GOSUB Tone_toggle
850 END IF
851 RETURN
852 Tune_toggle:
853 IF Tune=1 THEN
854 Tone=0 ON KEY 7 LABEL "Tune Mode OFF" GOSUB Tune_toggle
856 ELSE
857 Tune=1 ON KEY 7 LABEL "Tune Mode ON" GOSUB Tune_toggle
859 END IF
860 RETURN
861 Read_volt:
862 CALL Dv_read(1),Choice$(*),In_data(*))
863 STOP
864 Test_data:
865 ! DATA "xxxtest_dataxxx"
866 ! DATA "Sodium Spectra"
867 ! DATA "1.1,1.2,1.3,1.4,1.5,1.6"
868 ! Table: describing nomenclature...
869 ! DATA "123232","1 2 3","3"
870 ! DATA "500000","500100","500200","2","0"
871 ! DATA "xxxend_dataxxx"
872 ! DATA "Shaft Encoder","Scaler 1","Scaler 2"
873 ! DATA "A/D 0","A/D 1","A/D 2"
874 END:GCLEAR
875 OUTPUT 21,"K"
876 LOAD "MAC:HP913,703",1
877 END !-------------------------------------------------------------
878 !«««» ...................................................* ............* * * * * ............................................... .
879 !_ -_ - --------------------------------------------------------------------------------------------------------------------------
880 !---------------------------------------------------------------------------------------------------------------------------------
881 ! Subroutines Start here...
882 DEF FN_dev_on$<Group, Dev, Dev$> !-------------State if device is specified
883 T$=VAL$(Group>"A") &VAL$(Dev)
884 X=POS(Dev$,T$) IF X>0 THEN RETURN "Y" IF X<0 THEN RETURN "N"
885 END IF
886 FNEND
887 DEF FNChan_no<T$, Dev$> !------State if device is specified
888 CALL Unpack(Num_elements, Pack$(*), (Dev$)) IF T$="0.1" THEN
889 RETURN 0
890 GOTO 904
891 IF T$="LAST" THEN
892 RETURN Num_elements
893 GOTO 904
894 END IF
895 IF T$="0.1" THEN
896 NEXT I
897 IF Pack$<I>=T$ THEN X=I
898 RETURN X
305 SUB Dac_param(Desc$(*),Choice$(*))!
306 "Desc$(0)*="2"
307 FOR I=1 TO 2
308 READ Desc$(I)
309 READ Choice$(I)
310 NEXT I
311 DATA "Scalar 1 count time (sec)";"*";"Scalar 2 count time (sec)";"*
312 SUBEND
313 SUB Dac_read(Num_points,Choice$(*),Indata(*))!
314 DIM Bcd_data(15),Out_data(8)
315 IF FNDev_on$(1,2,Choice$(0))="Y" OR FNDev_on$(1,3,Choice$(0))="Y" THEN
316 CALL Go_count<VAL(Choice$(1)))
317 END IF
318 CALL Read_channels(Bcd_data(*),Out_data(*),Choice$(0))
319 IF FNDev_on$(1,7,Choice$(0))="Y" THEN CALL In_digidac(0,Out_data(7))
320 IF FNDev_on$(1,8,Choice$(0))="Y" THEN CALL In_digidac(0,Out_data(7))
321 IF Choice$(7)="Y" THEN CALL In_digidac(0,Out_data(7))
322 IF Choice$(8)="Y" THEN CALL In_digidac(0,Out_data(8))
323 D=1
324 FOR I=1 TO 8
325 IF FNDev_on$(1,1,Choice$(0))="Y" THEN
326 ! IF Choice$(I)="Y" THEN
327 XS="1."AVAL$(I)
328 Indata(FNChan_no<X$,Choice$(0),1)=Out_data(I)
329 END IF
330 NEXT I
331 SUBEND
332 SUB Dac_load ! LOAD SUB ALL FROM "DAC_DRIVE"
333 SUBEND
334 SUB Dac_purge ! DELSUB Setbit
335 DELSUB Resbit
336 DELSUB Makebit
337 DELSUB FNSigned
338 DELSUB Bcd_conv
339 DELSUB Read_channels
340 DELSUB Read_ad_channel
341 DELSUB In_digidac
342 DELSUB Out_digidac
343 SUBEND
344 SUB Go_count(Seconds)!
345 CALL Resbit(15) ! Reset Scalars
346 CALL Makebit(14,0) ! Unlatch displays
347 CALL Makebit(15,1) ! Start Counting
348 ON DELAY Seconds GOTO Latch_counter
349 Wait: GOTO Wait !And wait.
350 Latch_counter: GOTO Latch_counter !Stop Counters
351 CALL Makebit(14,1) ! Latch displays
352 SUBEND
353 SUB Bcd_conv(Bcd_data(*),Out_data(*)) !Convert entire block data
354 FOR J=0 TO 2
355 Temp=0
356 FOR I=1 TO 4+J*2
357 COSUB Byte_conv
358 Temp=Temp+Temp2
359 NEXT I
360 SUBEND
Out_data(J+1)=Temp
NEXT J
FOR J=0 TO 2
Temp=0
FOR I=2*J+9 TO 2*J+10
GOSUB Byte_conv
Temp=Temp+100+Temp2
NEXT I
Out_data(4+J)=Temp
NEXT J
SUBEXIT
Byte_conv: Temp2=BINAND(Bcd_data(I),240)*.625+BINAND(Bcd_data(I),15)
RETURN
SUBEND
SUB Setbit(Bit)
COM Gpio,Dev_control
Dev_control=BINOR(Dev_control,FNSigned(Bit))
SUBEND
SUB Resbit(Bit)
COM Gpio,Dev_control
Dev_control=BINAND(Dev_control,BINCMP(FNSigned(Bit)))
SUBEND
DEF FNSigned(Bit)
Value=2(Bit)
IF Value>32767 THEN Value=65536
RETURN Value
FMEND
SUB Makebit(Bit,Code) !SET BIT AS DIRECTED BY CODE
COM Gpio,Dev_control
IF Code=1 THEN
CALL Setbit(Bit)
ELSE
CALL Resbit(Bit)
END IF
CONTROL Gpio,3;Dev_control
SUBEND
SUB Read_channels(Bcd_data(1),Out_data(1),Dev$)------DAC READ
COM Gpio,Dev_control
CALL Makebit(14,1)
FOR Channel=0 TO 8
CONTROL Gpio,3;BINOR(Channel*16,Dev_control)
STATUS Gpio,3;Bcd_data(Channel)
NEXT Channel
CALL Resbit(15)
CONTROL Gpio,3;Dev_control
CALL Makebit(14,0)
FOR Chan=0 TO 2
IF FNSDev_on$(1,Chan,Dev$)="Y" THEN
CALL Read_ad_channel(Channel)
CONTROL Gpio,3;BINOR(9+Chan*2,Dev_control)
STATUS Gpio,3;Bcd_data(9+Chan+1)
CONTROL Gpio,3;BINOR(10+Chan*2,Dev_control)
STATUS Gpio,3;Bcd_data(10+Chan+1)
ELSE
Bcd_data(9+Chan*2)=0
Bcd_data(10+Chan*2)=0
END IF
FOR Chan=0 TO 2
CALL Bcd_conv(Bcd_data(1),Out_data(1))
SUBEND
SUB Read_ad_channel(Channel) !-------------------------A/D READ
CONTROL Gpio,Dev_control
162

Dev_control=BINAND(Dev_control--6145) !CLEAR CHANNEL
1027 Dev_control=BINEDR(Dev_control.2048=Channel) !SET NEW CHAN
1028 CALL Setbit(14) ;LATCH ALL DISPLAYS
1029 CALL Setbit(13) ;A/D ENABLE
1030 CALL Resbit(10) ;MPX DISABLE
1031 CALL Makebit(9,1) ;SAMPLE
1032 CALL Makebit(9,0) ;HOLD
1033 CALL Makebit(10,0)
1034 CALL Makebit(10,1) ;MPX ENABLE
1035 CALL Makebit(13,0) ;CONVERT
1036 CALL Makebit(13,1)
1037 CALL Makebit(14,1) ;UNLATCH
1038 SUBEND
1039 SUB Stepper_move(Control_param$(*)) !----------------------
1040 DIM Bcd_data(15),Out_data(8)
1041 COM Gpio,Dev_control
1042 Read_pos:
1043 FOR I=0 TO 2
1044 CALL Makebit(14,1)
1045 CONTROL Gpio_3:BINEDR(I+16,Dev_control)
1046 STATUS Gpio_3:Bcd_data(I)
1047 CALL Makebit(14,0)
1048 NEXT I
1049 CALL Bcd_conv(Bcd_data(*),Out_data(*))
1050 X=INT(VAL(Control_param$3))
1051 IF X-Out_data(1)>0 THEN DISP "Moving Grating to";X;" now at";Out_data(1)
1052 SELECT ABS(X-Out_data(1))
1053 CASE >10
1054 N=ABS(X-Out_data(1))
1055 FOR P=1 TO (N-5)+6
1056 GOSUB Move_one_step
1057 NEXT P
1058 WAIT .05
1059 GOTO Read_pos
1060 CASE >0
1061 GOSUB Move_one_step
1062 GOTO Read_pos
1063 CASE 0
1064 DISP
1065 GOTO Endsub
1066 END SELECT
1067 Move_one_step:
1068 IF Out_data(1)>X THEN
1069 CALL Setbit(0)
1070 CALL Makebit(1,0)
1071 CALL Makebit(1,1)
1072 ELSE
1073 CALL Resbit(0)
1074 CALL Makebit(1,0)
1075 CALL Makebit(1,1)
1076 END IF
1077 RETURN
1078 Endsub: Control_param$5=VAL$(Out_data(1))
1079 SUBEND
1080 SUB Stepper_control(Control_param$(*))
1081 Target=VAL(Control_param$3)
1082 Position=VAL(Control_param$5)
1083 Step=VAL(Control_param$4)
1084 Direction=SGN(VAL(Control_param$4))
1085 IF SGN(Target-Position)=Direction OR Position=0 THEN
1086 Control_param$$(3)=VAL$(Target-60+Direction)
1087 CALL Stepper1_move(Control_param$$(*)
1088 END IF
1089 Control_param$$(3)=VAL$(Target)
1090 CALL Stepper1_move(Control_param$$(*)
1091 End:Control_param$$(5)=Control_param$$(3)
1092 SUBEND
1093 SUB Window!
1094 COM /Parameters/ D(*) , Indev_parm$$(*) , Outdev_parm$$(*) , Devname$$(*) , Exp_controls$$(*) , Numparm
1095 COM /Param2/ Opname$$(80) , Dds$$(20) , Dfs$$(4) , Sid , Auto$$(10)(40)
1096 DIM Pack$$(10)(80) , Text$$(80) , Desc$$(18)(40) , Choice$$(18)(80)
1097 CLEARN
1098 FRAME
1099 Menu:PRINT TABXY(25,2);"Main Menu"
1100 OFF KEY
1101 ON KEY 5 LABEL "Return" GOTO Return
1102 PRINT TABXY(5,4);"A) Experiment Information"
1103 PRINT TABXY(5,5);"B) Scan Display Control"
1104 PRINT TABXY(5,7);"C) Post Scan Output Control"
1105 PRINT TABXY(5,9);"D) Experiment Control"
1106 PRINT TABXY(5,11);"E) Co-Addition Control"
1107 PRINT TABXY(5,13);"F) Device Specific Control"
1108 PRINT TABXY(5,15);"G) Save Parameters as Default"
1109 Maxi=7
1110 GOSUB Getline
1111 GOSUB Wipe_window
1112 X=1
1113 L1=1
1114 ON KEY 5 LABEL "Back Page" GOTO Menu_return
1115 ON X GOTO Info , Scan, Post_scan, Experiment, Co_add, Dev_spec, Save
1116 Menu_return:
1117 GOSUB Wipe_window
1118 L1=1
1119 GOTO Menu
1120 Info:
1121 Offset=0
1122 PRINT TABXY(25,2);"Experiment Information"
1123 PRINT TABXY(5,4);"A) Experiment Title":TAB(30);Exp_controls$$(1):TAB(60)
1124 PRINT TABXY(5,5);"B) Operator Name":TAB(30);Opname$:TAB(60)
1125 PRINT TABXY(5,6);"C) Data Drive Spec":TAB(30);Dds$:TAB(60)
1126 PRINT TABXY(5,7);"D) Data File Spec":TAB(30);Dfs$:TAB(60)
1127 PRINT TABXY(5,8);"E) Current Scan ID#":TAB(30);Sid:TAB(60)
1128 Maxi=5
1129 GOSUB Getline
1130 SELECT LI
1131 CASE 1
1132 LINPUT "Enter Experiment Title",Exp_controls$$(1)
1133 CASE 2
1134 LINPUT "Enter Operator Name",Opname$
1135 CASE 3
1136 LINPUT "Enter Valid Data Drive Spec",Dds$
1137 CASE 4
1138 LINPUT "Enter Data Filespec (4 characters max)",Dfs$[1:4]
1139 Dfs$=UPC$(Dfs$)
1140 CASE 5
1141 LINPUT "Current Scan ID number (4 digits)",Sid
1142 END SELECT
1143 GOTO Info
1144 Scan:
1145 Offset=11
1146 PRINT TABXY(25,2):"Display Control Menu"
1147 PRINT TABXY(5,4):"A) Assign Abscissa"
1148 PRINT TABXY(5,5):"B) Assign Ordinate"
1149 PRINT TABXY(5,6):"C) Auto Scaling"
1150 PRINT TABXY(5,7):"D) Manual Scaling"
1151 PRINT TABXY(5,8):"E) Printer Output"
1152 FOR I=11 TO 16
1153 PRINT TABXY(30,1-8);Exp_control$(I)
1154 NEXT I
1155 Max=5
1156 GOSUB Getline
1157 SELECT LI
1158 CASE 1,2
1159 DISP "Enter Device code. Current code=";
1160 DISP Exp_control$(LI+Offset);""
1161 INPUT Exp_control$(LI+Offset)
1162 CASE 3,5
1163 Op$="T"
1164 GOSUB Operator_input
1165 CASE 4
1166 INPUT "Enter Minimum Y value",Miny
1167 INPUT "Enter Maximum Y value",Maxy
1168 Exp_control$(15)=VAL$(Miny);"";VAL$(Maxy)
1169 CALL Unpack((0),Pack$(0),(Exp_control$(15)))
1170 END SELECT
1171 GOTO Scan
1172 Post_scan:
1173 Offset=16
1174 PRINT TABXY(25,2);"Post Scan Output"
1175 PRINT TABXY(5,4);"A) Save to Disk"
1176 PRINT TABXY(5,5);"B) Output to Plotter"
1177 PRINT TABXY(5,6);"C) Output to Printer"
1178 PRINT TABXY(5,7);"D) Run Time Status Line"
1179 PRINT TABX(5,8);"" to Printer?";
1180 PRINT TABX(30);Exp_control$(26);TAB(60)
1181 FOR I=17 TO 19
1182 PRINT TABXY(30,1-13);Exp_control$(I);TAB(60)
1183 NEXT I
1184 Max=4
1185 GOSUB Getline
1186 SELECT LI
1187 CASE 1,2,3
1188 Op$="I"
1189 GOSUB Operator_input
1190 CASE 4
1191 Offset=22
1192 Op$="T"
1193 GOSUB Operator_input
1194 END SELECT
1195 GOTO Post_scan
1196 Experiment:
1197 OFFSET
1198 ON KEY 5 LABEL "Back Page" GOTO Menu_return
1199 Offset=19
1200 PRINT TABXY(25,2);"Experiment Control Menu"
1201 PRINT TABXY(5,4);"A) Number of Scans"
1202 PRINT TABXY(5,5);"B) Pause Between Scan"
1203 PRINT TABXY(5,6);"C) Output Co-add when done"
1204 PRINT TABXY(5,7);"D) AutoScan Control"
1205 FOR I=20 TO 22
1206 PRINT TABXY(35,1-16);Exp_control$(I);TAB(60);
1207 NEXT I
1208 Max1=4
1209 GOSUB Getline
1210 SELECT LI
1211 CASE 1
1212 Op$="*"
1213 GOSUB Operator_input
1214 CASE 2.3
1215 Op$="T"
1216 GOSUB Operator_input
1217 CASE 4
1218 GOTO Autoscan
1219 END SELECT
1220 GOTO Experiment
1221 COAdd: 1
1222 Offset+22
1223 PRINT TABXY<25,2>:"Co-Addition Control"
1224 PRINT TABXY<5,4>:"A Assign X device"
1225 PRINT TABXY<5,5>:"B Assign Y device"
1226 PRINT TABXY<5,6>:"C Assign Relationship"
1227 FOR I=23 TO 25
1228 PRINT TABXY<30,15>;Exp_control$<I>;TAB<60>
1229 NEXT I
1230 Max1=3
1231 GOSUB Getline
1232 SELECT LI
1233 CASE 1,2
1234 DISP "Enter Device Code, Current code=';",
1235 DISP Exp_control$<L1+Offset>"
1236 INPUT Exp_control$<L1+Offset>
1237 CASE 3
1238 Op$="X/X/Y.X-Y.(X-Y)/Y""
1239 GOSUB Operator_input
1240 END SELECT
1241 GOTO Co_add
1242 Auto_scan: 1
1243 GOSUB Wipe_window
1244 PRINT TABXY<25,2>:"AutoScan Control"
1245 OFF KEY
1246 PRINT TABXY<10,13>:CHR$(129):"Use function keys to program AutoScan"
1247 R$(128)
1248 ON KEY 5 LABEL "Back Page" GOTO Quit
1249 ON KEY 6 LABEL "Set Limits" GOTO Limits
1250 ON KEY 7 LABEL "Set Step" GOTO Step
1251 ON KEY 8 LABEL "Set Delay" GOTO Delay
1252 ON KEY 9 LABEL "Scan" GOTO Doit
1253 ON KEY 0 LABEL "Delete last" GOTO Del
1254 N=VAL("0"&Auto$<0>)
1255 FOR I=1 TO N
1256 PRINT TABXY<4,12>;Auto$<I>;TAB<60>
1257 NEXT I
1258 PRINT TABXY<4,12>;TAB<60>
1259 L1:GOTO L1
1260 Limits:
1261 INPUT "Enter limits: From:"<,T
1262 INPUT "Enter limits: To:"<,X
1263 N=N+1
1264 Auto$<N>="Set Limits "&VAL$(T)&","&VAL$(X)
1265 GOTO 1255
1266 Step: 1
166

1267 INPUT "Enter number of units to step", T
1268 N=N+1
1269 Auto$(N)="Set Step "&VAL$(T)&" units"
1270 GOTO 1255
1271 Delay:
1272 INPUT "Enter seconds to delay between data points", T
1273 N=N+1
1274 Auto$(N)="Set Delay "&VAL$(T)&" seconds"
1275 GOTO 1255
1276 Doit:
1277 INPUT "Enter number of scans to take per cycle", T
1278 N=N+1
1279 Auto$(N)="Scan "&VAL$(T)&" times."
1280 GOTO 1255
1281 Wait2:
1282 INPUT "Enter WAIT duration in minutes", T
1283 N=N+1
1284 Auto$(N)="Wait "&VAL$(T)&" minutes"
1285 GOTO 1255
1286 Del:
1287 N=N-1
1288 IF N<0 THEN N=0
1289 GOTO 1255
1290 Quit: GOSUB Wipe_window
1291 Auto$(0)=VAL$(N)
1292 GOTO Experiment
1293 Dev_spec:
1294 Exp_control$(0)="1"
1295 OFF KEY
1296 GOTO 5 LABEL "Back Page" GOTO Menu_return
1297 PRINT TABXY(18,2):"Device Specific Information"
1298 PRINT TABXY(5,4):"Select Device:
1299 Op$="#"
1300 Offset=0
1301 L1=0
1302 GOSUB Operator_input
1303 SELECT Exp_control$(0)
1304 CASE "1"
1305 CALL Dac_parm(Desc$(0),Choice$(0))
1306 Tx=1
1307 CASE "3"
1308 CALL Dv_parm(Desc$(0),Choice$(0))
1309 Tx=3
1310 CASE ELSE
1311 GOTO Dev_spec
1312 END SELECT
1313 T$="ABCDEFGHIJKLMNOPQRSTUVWXYZ"
1314 FOR I=1 TO VAL(Desc$(0))
1315 PRINT TABXY(5,3+I);T$(I);" ";Desc$(I)
1316 NEXT I
1317 L1=1
1318 Dsloop:
1319 Maxi=VAL(Desc$(0))
1320 FOR I=1 TO Maxi
1321 PRINT TABXY(35,3+I);Indev_parm$(Tx,I)
1322 NEXT I
1323 GOSUB Getline
1324 Offset=-L1
1325 Exp_control$(0)=Indev_parm$(Tx,L1)
1326 Op$=Choice$(L1)
1327 GOSUB Operator_input
1328  Indev_parm$[Tx,L1]=Exp_control$(0)
1329  GOTO Dsloop
1330  Save:!
1331  OFF KEY
1332  PRINT TABXY(20,7);"Saving Default Values..."
1333  ASSIGN @Save TO "DACDEF"
1334  OUTPUT @Save;Exp_control$(*)
1335  OUTPUT @Save;Upnam$
1336  OUTPUT @Save;Dds$
1337  OUTPUT @Save;Dfs$
1338  OUTPUT @Save;VAL$(Sid)
1339  ASSIGN @Save TO *
1340  PRINT TABXY(20,7);"
1341  GOTO Menu
1342  Loop:GOTO Loop
1343  Getline:!
1344  DISP "Use Knob then press <space> (or press letter) for line to work on"
1345  IF LI=0 OR LI>Maxl THEN LI=1
1346  ON KNOB .1 GOTO Knob
1347  ON KBD GOTO Kbd
1348  PRINT TABXY(3,Li+3),";"
1349  Wait:GOTO Wait
1350  Knob:!
1351  PRINT TABXY(3,Li+3); ";
1352  Xx=KNOBX
1353  Dd=INT((ABS(Xx)+9)/10)*SGN(Xx)
1354  Li=Li+Dd
1355  IF Li>Maxl THEN Li=Maxl
1356  IF Li<1 THEN Li=1
1357  GOTO 1348
1358  Kbd:!
1359  PRINT TABXY(3,Li+3); ";
1360  AS=KBD$
1361  SELECT AS
1362  CASE " ~"
1363       LI=LI-1
1364  CASE " V"
1365       LI=LI+1
1366  CASE " E" " "
1367       OFF KBD
1368       OFF KNOB
1369       RETURN
1370  CASE ELSE
1371       Xs="ABCDEFGHIJKLMNOPQRSTUVWXYZ"
1372       L=POS(XS[1:Maxl],UPC$(AS))
1373       IF L>0 THEN
1374          Li=1
1375          OFF KBD
1376          OFF KNOB
1377       RETURN
1378       END IF
1379       END SELECT
1380       GOTO 1355
1381  Operator_input:!
1382  SELECT Ops
1383  CASE " T"
1384       IF Exp_control$(Offset+Li)="Y" THEN
1385          Exp_control$(Offset+Li)="N"
1386       ELSE
1387          Exp_control$(Offset+Li)="Y"
CASE 
    "#"
    INPUT "Enter Value",XS
    Exp_control$(Offset+L)+VAL$(VAL(X$))
CASE ELSE
    CALL Unpack(Num_elements, Pack$(*) , (Op$))
    X=0
    FOR I=1 TO Num_elements
        IF Exp_control$(Offset+L)-Pack$(I) THEN X=I
        NEXT I
    X=X+1
    IF X>Num_elements THEN X=1
    Exp_control$(Offset+L)-Pack$(X)
END SELECT
RETURN
Wipe_window:FOR I=14 TO 1 STEP -1
TO PRINT TABXY(1,1);RPT$=" " ,60):
NEXT I
RETURN
SUBEND
SUB Unpack(Num_elements, Pack$(*) , Text$)
    Num_elements=0
    DIM T2$(80)
    T2$=Text$
    Loop:L=LEN(T2$)
    X=POS(T2$",","" )
    IF LOOP THEN
        Num_elements=Num_elements+1
        Pack$(Num_elements)=T2$(X+1)
        IF X<1 THEN
            T2$=T2$[X+1]
        GOTO Loop
    END IF
END IF
SUBEND
SUB Pack(Num_elements, Pack$(*) , Text$)
    Text$=""
    FOR I=1 TO Num_elements
        Text$=" &Text$&Pack$(I)
    NEXT I
    Text$=Text$[2]
SUBEND
DEF FN3b$(Word)
    T$=VAL$(Word)
    Z$="000000"
    TS=Z$(1;8-LEN(T$))&T$
    Y$=""
    FOR I=0 TO 2
        Y$=Y$&CHR$(VAL(TS[I]*2+1))&16+VAL(TS[I]*2+1))
    NEXT I
    RETURN Y$
FNEND
DEF FNUnsigned_word(Word)
    IF Word<0 THEN Word=Word+65536
    RETURN Word
FNEND
SUB Dv_read(Num_points, Choice$(*), Indata(*))
    DIM A(1:100)
    GOSUB Read
GOTO 1456
1449 Read:S=SPOLL(722)
1450 DISP "Reading Voltmeter"
1451 FOR I=1 TO Num_points
1452 ENTER 722 USING ";K":Indata(FNChan_no(“3.1”,Choice$(0)),I)
1453 NEXT I
1454 DISP
1455 RETURN
1456 SUBEND
1457 SUB Dv_param(Desc$(*) ,Choice$(*)
1458 Desc$(0)="","
1459 FOR I=1 TO 2
1460 READ Desc$(I),Choice$(I)
1461 NEXT I
1462 DATA "Voltmeter Mode","DC Volts,AC Volts","Shift Functions","I"
1463 SUBEND
1464 SUB Dv_init(Num_points,Choice$(*)
1465 DIM X$[80]
1466 X$=""
1467 IF Choice$(1)="A" THEN-
1468 X$=X$&"F2 "
1469 ELSE
1470 X$=X$&"F1 "
1471 END IF
1472 IF Choice$(2)="Y" THEN
1473 X$=X$&"S1 "
1474 ELSE
1475 X$=X$&"S0 "
1476 END IF
1477 X$=X$&"GSTG 10ST1"
1478 OUTPUT 722:X$
1479 SUBEND
1480 SUB Lock_in_read(Num_points,Choice$(*) ,Indata(*))
1481 DIM Fsx[16]
1482 DISP "Reading Lock-In Amplifier"
1483 S9=SPOLL(712)
1484 IF BIT(S9,0)=0 THEN GOTO 1483
1485 OUTPUT 712:"TRIG 0"
1486 Pt=1
1487 FOR I=16 TO 2 STEP -2
1488 Fsx(I)=3*Pt
1489 Fsx(I-1)=1*Pt
1490 Pt=Pt/10
1491 NEXT I
1492 S9=SPOLL(712)
1493 IF BIT(S9,0)=0 THEN GOTO 1492
1494 OUTPUT 712:"SEN"
1495 ENTER 712:Fsx
1496 Fsx=Fsx+1
1497 FOR I=1 TO Num_points
1498 S9=SPOLL(712)
1499 IF BIT(S9,0)=0 THEN GOTO 1498 ! WAIT FOR PREVIOUS COMMAND DONE.
1500 OUTPUT 712:"OUT"
1501 S9=SPOLL(712)
1502 IF BIT(S9,7)=1 THEN GOTO 1504 ! CHECK OUTPUT READY BIT
1503 IF BIT(S9,0)=0 THEN GOTO 1501 ! WAIT FOR PREVIOUS COMMAND DONE.
1504 ENTER 712:
1505 Indata(FNChan_no(“4.1”,Choice$(0)),I)=(X/10000)*Fsx(Fsx)
1506 NEXT I
1507 DISP
1508 SUBEND
1509 SUB Lock_in5207_read(Num_points,Choice$(*) ,Indata(*))
1510 DIM Fs(21)
1511 DISP "Reading 5207 Lock-in Amplifier"
1512 J=0
1513 Pt=1.0
1514 FOR I=1 TO 19 STEP 3
1515 Fs(I)=5.0*Pt
1516 Fs(I+1)=2.0*Pt
1517 Fs(I+2)=1.0*Pt
1518 Pt=Pt/10
1519 NEXT I
1520 S9=SPOLL(713)
1521 IF BIT(S9,0)=0 THEN GOTO 1520
1522 OUTPUT 713;"S" ; FIND OUT WHAT VOLTAGE SCALE WE'RE ON
1523 ENTER 713:Fsi
1524 Fsi-Fsi+1
1525 FOR I=I TO Num_points
1526 S9=SPOLL(713) ; DO SERIAL POLL
1527 IF BIT(S9,0)=0 THEN GOTO 1526 ; WAIT FOR PREVIOUS COMMAND DONE
1528 OUTPUT 713;"Q1"
1529 S9=SPOLL(713) ; DO SERIAL POLL
1530 IF BIT(S9,7)=1 THEN GOTO 1532 ; CHECK OUTPUT READY BIT.
1531 IF BIT(S9,0)=0 THEN GOTO 1529 ; WAIT FOR PREVIOUS COMMAND DONE.
1532 ENTER 713:X
1533 Indata<FNChan_no("4.2",Choice$(0)),I>*(X/2000)*Fs(Fs1)
1534 NEXT I
1535 DISP
1536 SUBEND
1560 SUB Dumper(Xlim,Ylim,Comment$)
1561 INTEGER G(7700)
1562 DIM W$(400)
1563 GSTORE G(»)
1566 Xx=Xlim
1567 Yy=Ylim
1568 T1=TIME$DATE
1569 INTEGER R,B,L,K,X,Y,Z
1570 OUTPUT 701;CHR$(27);"*1D";
1571 FOR I=0 TO Yy*25 STEP 200
1572 OUTPUT 701;CHR$(27);"b";VAL$(Xlim);"G";
1573 FOR X=0 TO Xx/16-1
1574 X2=X/16
1575 FOR Z=0 TO 15
1576 B=0
1577 FOR K=0 TO 7
1578 B=BINOR(B,SHIFT(BIT(G(I+K*25+X).15-Z). K-7))
1579 NEXT K
1580 OUTPUT 701;CHR$(B);
1581 NEXT Z
1582 OUTPUT 701;""
1583 IF I=12.5 AND Flag=0 THEN
1584 OUTPUT 701:Comment$;
1585 Flag=1
1586 END IF
1587 OUTPUT 701;""
1588 NEXT I
1590 OUTPUT 701;CHR$(27);"16D";
1592 SUBEND
1600 SUB Dumper(Xlim,Ylim,Comment$)
1601 INTEGER G(7700)
1602 DIM W$(400)
1603 GSTORE G(»)
1606 Xx=Xlim
1607   Yy=Ylim
1608   T1=TIMEDATE
1609   INTEGER R,B,L,K,X,Bs,Z
1610   OUTPUT 701;CHR$(27);"&19D";
1611   FOR I=0 TO Yy=25 STEP 200
1612   OUTPUT 701;CHR$(27);"b";VAL$(Xlim);"G";
1613   FOR X=0 TO Xx/16-1
1614   X2=X*16
1615   FOR Z=0 TO 15
1616   B=0
1617   FOR K=0 TO 7
1618       B=BINEOR(B,SHIFT(BIT(G[I+K*25+X],15-Z),K-7))
1619   NEXT K
1620   NEXT Z
1621   NEXT X
1622   IF I>Yy=12.5 AND Flag=0 THEN
1623       OUTPUT 701;Comment$;
1624       Flag=1
1625   END IF
1626   OUTPUT 701;"
1627   NEXT I
1628   OUTPUT 701;CHR$(27);"&16D";
1629   SUBEND
1630   SUB Dumper(Xlim,Ylim,Comments)
1631   INTEGER G(7700)
1632   DIM WS(400)
1633   GSTORE G(*)
1634   Xx=Xlim
1635   Yy=Ylim
1636   T1=TIMEDATE
1637   INTEGER R,B,L,K,X,Bs,Z
1638   OUTPUT 701;CHR$(27);"&19D";
1639   FOR I=0 TO Yy=25 STEP 200
1640   OUTPUT 701;CHR$(27);"b";VAL$(Xlim);"G";
1641   FOR X=0 TO Xx/16-1
1642   X2=X*16
1643   FOR Z=0 TO 15
1644   B=0
1645   FOR K=0 TO 7
1646       B=BINEOR(B,SHIFT(BIT(G[I+K*25+X],15-Z),K-7))
1647   NEXT K
1648   NEXT Z
1649   NEXT X
1650   IF I>Yy=12.5 AND Flag=0 THEN
1651       OUTPUT 701;Comment$;
1652       Flag=1
1653   END IF
1654   OUTPUT 701;"
1655   NEXT I
1656   OUTPUT 701;CHR$(27);"&16D";
1657   SUBEND
APPENDIX B

MODIFIED OVERLAY PROGRAM SECTION TO CREATE ASCII FILES
GOTO New_screen

Overlay: !

INPUT "Specify: 'NULL', 'CURRENT', 'SCAN', or a valid File name", XS

SELECT XS

CASE "NULL"; "" ! ANY OVERLAYS ARE CANCELLED.

Overlay=0

CASE "CURRENT" ! TURNS BACK ON AN OVERLAY FILE "NULL" TURNED OFF.

Overlay=1

CASE "SCAN" ! PUTS CURRENT SCAN INTO OVERLAY ARRAYS.

X=FNChan_no(Exp_control$<12>,Exp_control$<2>)

Y=FNChan_no(Exp_control$<13>,Exp_control$<2>)

FOR I=1 TO 4096

OvI(I,1)=OvI(X)

OvI(I,2)=OvI(Y)

NEXT I

CASE ELSE ! RETRIEVES A FILE FROM DISK TO BE OVERLAID.

Dds$=":INTERNAL,4,1"

Ddo$=":INTERNAL,4,0"

OvI$=XS

CREATE ASCII OvI$4Ddo$,35

1 IF Exp_control$<12>="2.1" THEN

R$="R"

CASE "R","r"

CASE "S","s"

CASE "SD","sd"

CASE "C","c"

CASE ELSE

INPUT "LAST SCAN TO BE CO-ADDED? (Y OR N)?", XS

IF XS="N" THEN GOTO 774

IF XS="Y" THEN GOTO 763

INPUT "ENTER TOTAL # OF SCANS.", Ns

CASE "Y","t"

CASE ELSE

GOTO 748

END SELECT

END IF

ON ERROR GOTO Diskin_error

ASSIGN @Input TO OvI$4Dds$

ASSIGN @Output TO OvI$4Ddo$

OFF ERROR

ENTER @Input; T$ ! Title of old file

ENTER @Output; T$ ! Input devices of old file

OvI=FNChan_no(Exp_control$<12>,T$)

Ov2=FNChan_no(Exp_control$<13>,T$)

Ns=FNChan_no("LAST",T$)
ENTER Input;TS
N=VAL(TS[POS(TS,"."),POS(TS,""))+1)}
ENTER Input;TS
Entered sequence no. and # elements
ENTER Input;TS
Date and time
ENTER Input;TS
Operator Name
ENTER Input;TS
ENTER Input;TS
ENTER Input;TS
ENTER Input;TS
ENTER Input;TS
ENTER Input;TS
FOR i=1 TO N-1
IF I/5=INT(I/5) THEN
DISP "Loading in file ";Ovl$; " Record: ";I; "of ";N
END IF
IF Exp_control$(12)="2.1" THEN GOTO 802
FOR J=1 TO Nc
ENTER Input;X
IF J-Ovl THEN Ovl(I,1)=X ! ABSCISSA DATA
IF J-Ov2 THEN Ovl(I,2)=X ! ORDINATE DATA
NEXT J
GOTO 823
802 X-FNChan_no"2.1", Exp_control$$(2))
Y-FNChan_no"4.2", Exp_control$$(2))
R-FNChan_no"4.2", Exp_control$$(2))
ENTER Input;Ovl(I,X),Ovl(I,Y),Ovl(I,R)
806 IF R$="R" THEN Ovl(I,Y)=Ovl(I,Y)/Ovl(I,R) ! DIVIDE CURRENT BY OVERLAY
807 IF R$="S" THEN GOTO 823 ! STRAIGHT INPUT
808 IF R$="SD" THEN
809 D(I,X)=Ovl(I,X)
810 D(I,Y)=Ovl(I,Y)
811 D(I,R)=Ovl(I,R)
812 OUTPUT Output;D(I,X),D(I,Y),D(I,R)
813 END IF
814 IF R$="C" THEN
815 D(I,Y)=D(I,Y)+Ovl(I,Y)
816 IF Ns>1 THEN D(I,Y)=D(I,Y)/Ns
817 END IF
818 IF R$="T" THEN Ovl(I,Y)=Ovl(I,Y)/D(I,Y) ! DIVIDE OVERLAY BY CURRENT
819 NEXT I
820 OUTPUT Output;Ovl(0,0)=N-1
821 Overlay=1
822 IF R$="SD" THEN
823 Overlay=0
824 D_element=N
data$=Ovl$(1:4)
825 Sيد=VAL(data$$(5,9))
826 END IF
827 ASSIGN Input TO *;
828 END SELECT
829 GOTO New_screen
830 GOTO Screen_draw
831 Diskin_error!
832 DISP "Bad file ";FS:
833 GOTO Overlay
834 Tone_toggle:
835 IF Tone=1 THEN
836 Tone=0
837 ELSE
838 Tone=1
839 ON KEY 2 LABEL "Tone is ON" GOSUB Tone_toggle
LIST OF REFERENCES


10. Figure 1 was supplied by JPL to K. Narahari Rao 8/15/89.


54. Private communication L.S. Rothman and R.A. Toth.


