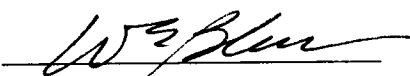


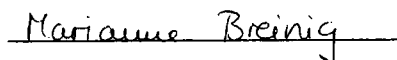
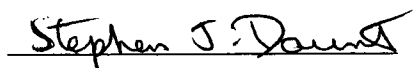
To the Graduate Council:

I am submitting herewith a thesis written by Larry W. Jennings entitled "Spectroscopic Studies of Ethylene and Methyl Cyanide Intensities". I have examined the final copy of this thesis for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Physics.



W. E. Blass, Major Professor

We have read this thesis and
recommend its acceptance:



Accepted for the Council:



Associate Vice Chancellor

and Dean of the Graduate School

STATEMENT OF PERMISSION TO USE

In presenting this thesis in partial fulfillment of the requirements for a Master's degree at the University of Tennessee, Knoxville, I agree that the Library shall make it available to borrowers under rules of the Library. Brief quotations from this thesis are allowable without special permission, provided that accurate acknowledgments of the source is made.

Permission for extensive quotation from or reproduction of this thesis may be granted by my major professor, or in his absence, by the Head of the Interlibrary Services when, in the opinion of either, the proposed use of the material is for scholarly purposes. Any copying or use of the material in this thesis for financial gain shall not be allowed without my written permission.

Signature Larry W. Jennings

Date 12/2/94

Spectroscopic Studies of Ethylene and
Methyl Cyanide Intensities

A Thesis

Presented for the

Master of Science

Degree

The University of Tennessee, Knoxville

Larry W. Jennings

December 1994

ACKNOWLEDGMENTS

Several people have made it possible for me to complete my graduate studies. Their assistance and guidance have been greatly appreciated. I would like to thank my advisor, Dr. William E. Blass, for sharing his knowledge of Molecular Spectroscopy and always making time to talk to me. I would also like to thank Dr. Stephen J. Daunt for making my stay at the University of Tennessee Molecular Spectroscopy Lab an enjoyable one and also for being a good friend. I also would like to thank Dr. Marianne Breinig for agreeing to be on my thesis committee and for helping me throughout my graduate study. Without these three, I would not be writing this thesis.

A special thanks to my friends at the University of Tennessee with whom I have shared many wonderful times. Thanks to Stewart Hager, John Lewis, Larry Senesac and Alan Ewing for their friendship and assistance. A special thanks to Gerald McElyea for technical assistance and being willing to help me even when he did not have time. I will always be indebted to him. I would also like to acknowledge the aid of Dr. Tom Callcott and his graduate student, Ling Zhou, for coating several mirrors needed in my experimental design. They worked hard for several weeks to get them done. And Dr. James Parks for his support and looking out for me. I would also like to thank my good friends, Glenna Odham and Robin Lucas for their friendship and for making time to listen when I needed to talk. And to my brother, Keith, thanks for all the golf and the laughs. Looks like I finally made it, brother.

Finally, I would like to thank the two people who made all of this possible, my parents, Wayne and Eula Jennings. They have watched me grow up and finally reach the one dream that I have had for a long time. Without their love and understanding, none of this would have been worthwhile.

ABSTRACT

Spectra of the ν_7 band of ethylene and the ν_7 and ν_4 bands of methyl cyanide were taken using the tunable diode laser (TDL) spectrometer at the University of Tennessee Molecular Spectroscopy Laboratory. The data were analyzed to determine absorption line intensities (strengths). The vibration-rotation spectra were acquired using a 48.26 cm absorption cell and pressures from 15 to 100.3 milliTorr for the ethylene data. The methyl cyanide spectra were obtained using a White cell with a path length of 825 cm and pressures of 61 to 601 milliTorr. In addition, absorption line strengths were determined using Fourier transform spectrometer data from the Kitt Peak National Observatory obtained from John Hillman of NASA's Goddard Space Flight Center. The FTS line strengths were scaled using results from the TDL line strength measurements. Transition line frequencies were determined for the ν_7 and $3\nu_8^1$ vibration-rotation bands of methyl cyanide. These results were obtained using the FTS data. Calibration of the transition line frequencies was performed using ethylene absorption lines present in the spectra.

TABLE OF CONTENTS

Introduction	Justification of Research	1
	Overview	1
	Methyl Cyanide	2
	Ethylene	6
Chapter 1	Theory of Symmetric and Asymmetric Molecules	8
	Symmetric Rotor	9
	Asymmetric Rotor	11
Chapter 2	Experimental Setup	15
	Overview	15
	UTMSL Tunable Diode Laser Spectrometer	15
	Experimental Procedure	27
	Recent Experimental Design Change	30
Chapter 3	Experimental Results	34
	Overview	34
	FTS Data, Transition Assignments	34
	Method of Analysis	36
	Calibration of Methyl Cyanide Energies	37
	Ground State Combination Differences	37
	TDL Intensity Measurements	51
	Intensity Analysis of TDL Data	54
	Methyl Cyanide Intensities	54
	Ethylene Intensities	58
Chapter 4	Future Work and Comparison of Results	61
	Future Work on Methyl Cyanide and Ethylene	61
	Comparison to Recent Results	62
	Conclusion	63
List of References		64
Appendices		68
	Appendix A	69
	Appendix B	106
	Appendix C	134
	Appendix D	135
	Appendix E	137
Vita		140

LIST OF TABLES

Table	Caption	Page
0.1	Bands and frequencies for Methyl Cyanide	3
1.1	Moments of Inertia Representations	12
2.1	Grating calibration data	26
3.1	Ethylene Absorption Line Energies in Wavenumbers from calibrated KPNO Ethylene Spectra and uncalibrated (observed) KPNO Methyl Cyanide Spectra	38
3.2	Molecular constants used to calculate ground state energies	40
3.3	Calculated and Observed $^RQ_0$ assignments in wavenumbers	46
3.4	Methyl Cyanide Pressure Broadening Data for Absorption Data at 1010.46 cm^{-1}	55
3.5	Methyl Cyanide Intensities from TDL Absorption Spectra	57
3.6	Stengths from TDL and recalibrated FTS data for ethylene absorption lines. Errors in strengths are standard deviations and are given parenthetically in the last digits of the strengths. $\langle S \rangle$ are averages of the S_{EW} and S_{τ} . Strengths are scaled to 296 K.	59
4.1	Comparison of absorption line strengths. Errors, where available, are given in parenthesis. Strengths are given in units of $\text{cm}^{-2}\text{ atm}^{-1}$ and ν_0 is in wavenumbers.	62
A.1	Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN	69
C.1	Methyl Cyanide TDL Absorption Spectrum Preliminary Data Results	134
D.1	Ethylene TDL Absorption Spectrum Preliminary Data Results	135
E.1	Ethylene Absorption Line Strengths from FTS Data	137

LIST OF FIGURES

Figure	Caption	Page
0.1	Observed emission lines from Sagittarius B2	4
0.2	Observed transitions for $J = 12 \rightarrow 11$ in OMC1	5
2.1	TDL Manifold Pumping System	18
2.2	Main TDL Optical Diagram	19
2.3	White cell pressure increase curve	21
2.4	TDL Optical Diagram with White Cell	22
2.5	White cell optical path, 4 m path shown	24
2.6	Positions of images on white cell mirror for 8 m path length	24
2.7	Wide TDL scans with top scan showing CH_3CN only, middle scan showing CH_3CN and C_2H_4 , and corresponding etalon scan on bottom. The two arrows point to two strong C_2H_4 lines.	29
2.8	Narrow TDL scan of C_2H_4 with etalon scan overlapped. C_2H_4 line is at $951.73787 \text{ cm}^{-1}$.	31
2.9	New optical design of TDL system	32
3.1	Sample DECOMP screen showing the $^R\text{Q}_0$ branch of CH_3CN	35
3.2	Methyl Cyanide Calibration Curve	39
3.3	GSCD Level Scheme	42
3.4	Sample GSCD Calculations	43
3.5	$^R\text{R}_0(J)$ transition energies vs m number graph	44
3.6	Example Q branches from CH_3CN spectrum	48
3.7	Definition of Equivalent Width	53
3.8	Methyl Cyanide Pressure Broadening Curve	56
3.9	Ethylene FTS Strength Calibration Curve	60

Introduction

Justification of Research

Overview

The principal focus of this work is a study of methyl cyanide, CH_3CN , its transition frequencies in wavenumbers ($\text{cm}^{-1} = \text{Hz}/c$ where c is the speed of light, a defined physical empirical constant), intensities and collision broadening coefficients in the $10\text{ }\mu\text{m}$ region. In order to pursue this study, experimental modifications and extensions to the UTMSL (University of Tennessee Molecular Spectroscopy Laboratory) TDL (tunable diode laser) spectrometer were required. These experimental efforts form a central part of this study. A secondary goal, related but separate, was to validate and extend the ethylene, C_2H_4 , intensity determinations made by Alan Ewing (Ewing, Alan, Masters thesis, University of Tennessee, 1993) and Dennis C. Reuter et al. (Reuter, D. and J. M. Sirota, *Absolute Intensities and Foreign Gas Broadening Coefficients of the $11_{1,10} \leftarrow 11_{2,10}$ and $18_{0,18} \leftarrow 18_{1,18}$ Lines in the ν_7 Band of C_2H_4* , **Journal of Quantitative Spectroscopic Radiative Transfer**, Vol. 50, No. 5, p. 477-482, 1993). The immediate goal of the ethylene study is to make possible the normalization (i.e., calibration) of line strengths retrieved from a broad-band, high resolution spectral study of ethylene made by John Hillman et al. using the KPNO (Kitt Peak National Observatory) NSO (National Solar Observatory) McMath Solar Telescope FTS (Fourier Transform Spectrometer). Once this calibration is complete it will be possible to complete a very important spectral atlas of $10\text{ }\mu\text{m}$ ethylene for use in extraterrestrial studies of atmospheres (Blass, W. E., S. Daunt, A. Ewing, S. Hager, J. Hillman, D. Jennings, L. Jennings, D. Reuter, L. Senesac, and M. Weber, **An Ethylene Atlas**, to be published, 1995).

The experimental modification and extensions are complete and methyl cyanide broadening has been measured. Preliminary intensity data on methyl cyanide were taken but are limited by a problem with the TDL system, so the methyl cyanide intensity measurements provide proof of capability to make the

intensity measurements. The TDL problem has subsequently been resolved. The extension and validation of ethylene intensities was carried out on the revitalized TDL system and results are presented.

Methyl Cyanide

Astronomers have detected methyl cyanide in molecular clouds, planetary atmospheres, and possibly comets. In order to identify the presence of molecules by analyzing absorption or emission spectra, exact line transition frequencies must be known. These transition frequencies act as the fingerprints of the molecules. Line intensities are needed to aid in the determination of pressures and temperatures of the gases from observational data and to make it possible for planetary atmosphere modeling to be accomplished.

Methyl cyanide is a symmetric rotor molecule with a large dipole moment ($\mu = 3.9$ debye). It belongs to the C_{3v} symmetry group. The number of modes associated with this molecule can be determined from the equation for the internal vibrational degrees of freedom

$$\text{Normal Modes} = 3N - 6 \quad (0.1)$$

where N is the number of atoms in the molecule. For methyl cyanide, $N = 6$ giving a total of 12 normal modes, some degenerate and some non-degenerate. Group theory can be used to determine the different modes and effects on the bonds. Table 0.1 (Duncan, J. L., *The calculation of force constants and normal coordinates* — *V*, *Spectrochimica Acta*, Vol. 20, p. 1197, 1964.) shows 8 fundamental modes or bands associated with methyl cyanide and their wavenumber region.

Transition energy assignments have been made by Parker et al. (Parker, F. W., A. H. Nielsen, and W. H. Fletcher, *The Infrared Absorption Spectrum of Methyl Cyanide Vapor*, **Journal of Molecular Spectroscopy**, **1**, 107-123, 1957.) at low resolution and Mori et al. (Mori, Y., T. Nakagawa, and K. Kuchitsu, *Vibration-Rotation Spectra of CH₃CN: The ν_7 Band and Its Hot Bands near 1040 cm⁻¹*, **Journal of Molecular Spectroscopy**, **104**, 388-401, 1984.) at 0.06 cm⁻¹ resolution and recently by

Table 0.1

Bands and frequencies for Methyl Cyanide

Band	Frequency (cm ⁻¹)
ν_1	2926
ν_2	2265
ν_3	1393
ν_4	921
ν_5	3033
ν_6	1461
ν_7	1040
ν_8	365

Tolonen et al. (Tolonen, A.-M., M. Koivusaari, R. Paso, J. Schroderus, S. Alanko, and R. Anttila, *The Infrared Spectrum of Methyl Cyanide between 850 and 1150 cm⁻¹: Analysis of the ν_4 , ν_7 , and $3\nu_8^1$ bands with Resonances*, **Journal of Molecular Spectroscopy**, **160**, 554-565, 1993.) at a resolution of 0.0035 cm⁻¹. No published work on methyl cyanide line intensities has been found in the literature. Microwave studies have determined a large self broadening coefficient (Swindle, D. J., and J. A. Roberts, *Linewidth*

Parameters in the Rotational Spectrum of Methyl Cyanide, Journal of Molecular Spectroscopy, 77, No. 1, July 1979).

The fact that methyl cyanide spectra contain lines that have relatively large energies separating them and that there are many lines that can be observed in a single scan makes methyl cyanide a valuable tool in determining temperatures, velocities and density estimates of the gases in the environment in which it is found. Solomon et al. (Solomon, P. M., K. B. Jefferts, A. A. Penzias, and R. W. Wilson, *Detection of Millimeter Emission Lines from Interstellar Methyl Cyanide*, **The Astrophysical Journal**, 168, L107-110, 1971) reported methyl cyanide present in the Sagittarius B and Sagittarius A molecular clouds in the 2.7 mm region. The lines were remeasured by Solomon, et al. (Solomon, P. M., A. A. Penzias, K. B. Jefferts, and R. W. Wilson, *Millimeter Emission Lines of Polyatomic Molecules in Sagittarius B2*, **The Astrophysical Journal**, 185, L63-L66, 1973) with better resolution. From their measurements an estimate of the kinetic temperature of the cloud could be made (100 K) and a density estimate of the molecule could be calculated. Figure 0.1 shows their observational data of the ground vibrational state ($J = 0$ to $J = 1$) from the Sagittarius B2 cloud.

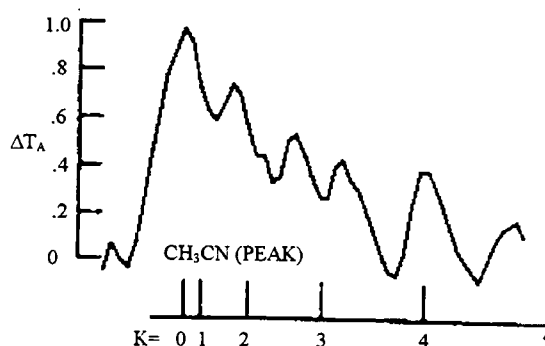


Figure. 0.1

Observed emission lines from Sagittarius B2

In addition Clark, et al. (Clark, F. O., R. D. Brown, P. D. Godfrey, J. W. V. Storey, and D. R. Johnson, *Detection of Interstellar Vibrationally Excited Cyanoacetylene*, **The Astrophysical Journal**, 210, L139-L140, 1976) detected a broad line at 92.3527 GHz in the Orion molecular cloud that is believed to be from the ν_8 band of methyl cyanide. Loren, et al. (Loren, R. B., L. Mundy, and N. R. Erickson, *High Temperature Methyl Cyanide in Orion Molecular Cloud I*, **The Astrophysical Journal**, 250, 573-578, 1981) measured several lines from which they were able to determine the temperature of the cloud and also velocities of different areas of the cloud. Figure 0.2 shows their data for the $J = 12 \rightarrow 11$ transition at frequencies of approximately 220 GHz from the rotational state, ν_0 .

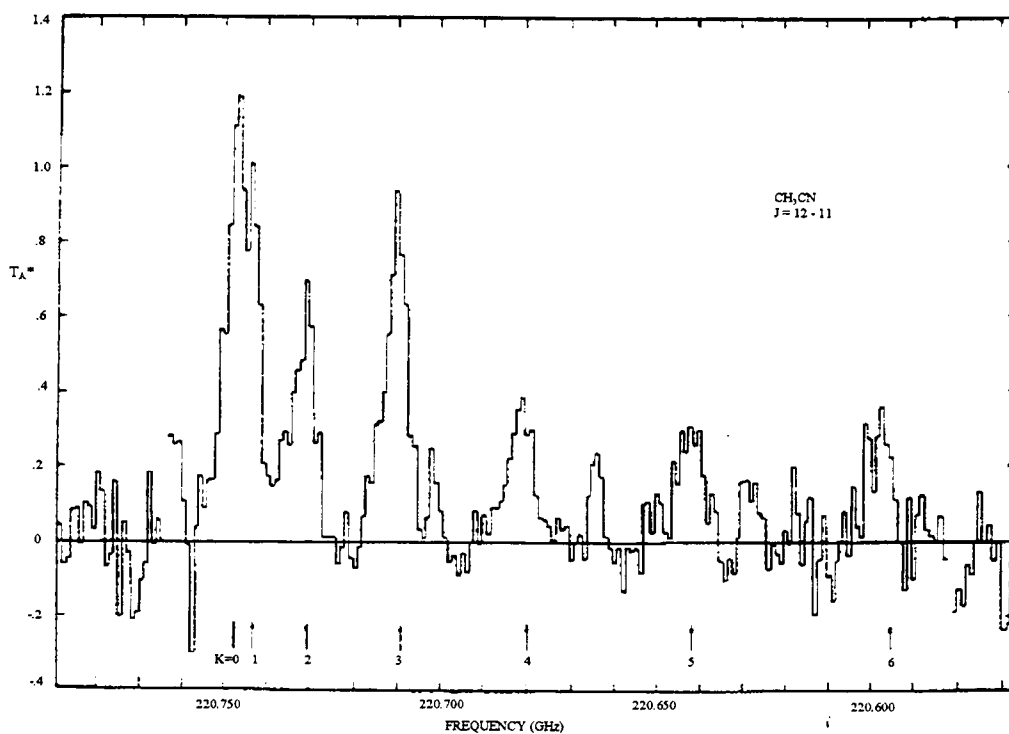


Figure 0.2

Observed transitions for $J = 12 \rightarrow 11$ in OMC1.

Methyl cyanide has been found in air samples near ground level (Becker, K. H. and A. Ionescu, *Acetonitrile In The Lower Atmosphere*, **Geophysical Research Letters**, Vol. 9, No. 12, p. 1349—1351, 1982.) at various locations in Europe. The concentration of methyl cyanide in the atmosphere was found to increase after burning grass and bushes and increases may also be caused by some industrial emissions. The data also shows a possible increase in concentration in urban areas over rural areas due to, in particular, car emissions. Methyl cyanide was also measured in the atmosphere in the United States by Snider and Dawson (Snider, J. R. and G. A. Dawson, *Surface Acetonitrile Near Tucson, Arizona*, **Geophysical Research Letters**, Vol. 11, No. 3, p.241—242, 1984). An increase in methyl cyanide may increase the amount of methane, CH₄, in the stratosphere. Arnold et al. (Arnold, F., H. Böhringer, and G. Henschen, *Composition Measurements of Stratospheric Positive Ions*, **Geophysical Research Letters**, Vol. 5, No.8, p. 653—656, 1978) speculate that methyl cyanide is present in the earth's stratosphere. Their experimental observations were made at a height of 33—37 km using a balloon born mass spectrometer. However, an infrared study of the atmosphere by Muller (Muller, C., *Acetonitrile in the Earth's Atmosphere: An Upper Limit Deduced from Infrared Solar Spectra*, **Bull. Cl. Sc. Acad. Roy. Belg.**, p. 225—229, 1985) is inconclusive in the identification of methyl cyanide.

Ethylene

The ethylene study is important to planetary science studies. A good review is given by Ewing (Alan Ewing, p. 4-6). Ethylene is present in the atmosphere of earth due primarily to car emissions. In addition to this, natural sources of ethylene are forest fires, volcanoes and plants (Abeles, F. B. and H. E. Heggstad, *Ethylene: An Urban Air Pollutant*, **Journal of Air Pollution Control Association**, 23, 517, 1973). Ethylene reacts with other molecules in the atmosphere and by receiving energy from the sun is able to form other compounds. Formaldehyde (H₂CO) and nitrous oxide (NO₂) are most common (Alan Ewing, p.4).

Ethylene has been detected in the atmosphere of Titan (Strobel, D. F., *The Photochemistry of Hydrocarbons in the Atmosphere of Titan*, **Icarus**, **21**, 466, 1974) and Jupiter (Kostuik, T., F. Espenak, M. Mumma, and P. Romani, *Infrared Studies of Hydrocarbons on Jupiter*, **Infrared Physics**, **29**, 198-204, 1989). Ethylene is expected to be present in any atmosphere which contains methane gas. Spectra taken of Titan by Voyager yielded features at the 940 cm^{-1} region. These were assigned to the ν_7 Q branch (Gillett, F. C., *Further Observations of the 8-13 Micron Spectrum of Titan*, **The Astrophysical Journal**, **201**, L41-L43, 1975), (Maguire, W. C., R. A. Hanel, D. E. Jennings, V. G. Kunde and R. E. Samuelson, **Nature**, **292**, 683-686, 1981). Jupiter also has ethylene present in its atmosphere but due to the presence of ammonia, the ν_7 band of ethylene is difficult to observe. Ethylene is expected to be present in the atmospheres of Saturn and Neptune.

The star IRC + 10216 has a circumstellar cloud surrounding it that was discovered to have ethylene (Betz, A. L., *Ethylene in IRC +10216*, **The Astrophysical Journal**, **244**, L103-L105, 1981) lines from the ν_7 band. By studying this cloud, Betz was able to determine a rate of expansion, temperature and radial column density. Further intensity measurements of earth based, laboratory spectra of ethylene would make it possible to make better temperature and density determinations.

The goal of an active collaboration between LEP (Laboratory for Extraterrestrial Physics) at GSFC (Goddard Space Flight Center) and UTMSL is an ethylene spectral atlas for planetary atmosphere modeling (Blass, W. E. and J. Hillman, private communication).

Chapter 1

Theory of Symmetric and Asymmetric Molecules

In order to pursue this study, it was necessary to become conversant with the broad and complex area of vibration and rotation energies of symmetric and asymmetric molecules. A brief summary of the zero order quantum mechanical Hamiltonian and rigid molecule energy levels for symmetric and asymmetric molecules is presented.

The total energy of a molecule can be expressed as (Daunt, Stephen, Ph.D. dissertation, Queen's University, Canada, 1976)

$$E_{\text{total}} = E_{\text{translational}} + E_{\text{electronic}} + E_{\text{vibration}} + E_{\text{rotation}} + E_{\text{translation-rotation}} + E_{\text{rotation-vibration}} + E_{\text{translation-vibration}} \quad (1.1)$$

In the Born-Oppenheimer approximation (Cohen-Tannoudji, C., B. Diu, and F. Laloe, Quantum Mechanics, Vol. I, p. 512, Wiley & Sons, New York, 1977), the motion of the electrons is treated separately from the motion of the nuclei. Fixing the center of mass of the molecule, one can then write the rotation-vibration energy of the nuclei as

$$E_{\text{rov}} = E_{\text{rotation}} + E_{\text{vibration}} + E_{\text{rotation-vibration}} \quad (1.2)$$

The Hamiltonian for the nuclear motion is

$$H_{\text{rov}} = T_{\text{rov}} + V_{\text{rov}} = H_{\text{rot}} + H_{\text{vib}} + H_{\text{rot-vib}} \quad (1.3)$$

Symmetric Rotor

The kinetic energy for a rigid rotor in its most basic form can be written as

$$2T = I_{xx}\omega_x^2 + I_{yy}\omega_y^2 + I_{zz}\omega_z^2 \quad (1.4)$$

where I is the moment of inertia tensor and ω is the rotation of the molecule about an axis. For a symmetric rotor (top), two moments of inertia are equal so we have, for instance

$$I_{xx} = I_{yy} = I_{\perp} \quad (1.5)$$

$$I_{zz} = I_{//} \quad (1.6)$$

In order to write the Hamiltonian, the kinetic energy must be in terms of momentum and by using

$$J_{qq} = I_{qq}\omega_q \quad (1.7)$$

the Hamiltonian can be written as

$$H = \frac{1}{2I_{\perp}}(J_x^2 + J_y^2) + \frac{1}{2I_{//}}J_z^2 \quad (1.8)$$

$$\text{and since } J^2 = J_x^2 + J_y^2 + J_z^2 \quad (1.9)$$

the Hamiltonian becomes

$$H = \frac{1}{2I_{\perp}}(J^2 - J_z^2) + \frac{1}{2I_{//}}J_z^2 \quad \text{or} \quad (1.10)$$

$$H = \frac{1}{2I_{\perp}}J^2 + \left(\frac{1}{2I_{//}} - \frac{1}{2I_{\perp}}\right)J_z^2. \quad (1.11)$$

Using

$$\langle jk | J^2 | jk \rangle = J(J+1)\hbar^2 \quad (1.12)$$

$$\langle jk | J_z | jk \rangle = K\hbar \quad (1.13)$$

one diagonalizes H, yielding the rigid rotor energy

$$E = BJ(J+1) + (A-B)K^2 \quad (1.14)$$

where

$$A = \frac{\hbar^2}{2I_{//}} \quad (1.15)$$

and

$$B = \frac{\hbar^2}{2I_{\perp}} \quad (1.16)$$

The rigid molecule energy is, however, a simple approximation. If one takes into account that the molecule is non-rigid, then additional terms are required to predict line energies. When the molecule is

rotating, the interatomic distances become longer and this causes a slight but measurable difference in the energy levels. The energy equation becomes

$$E_v(J, K) = B_v J(J+1) + (A_v - B_v)K^2 - D_J^v J^2(J+1)^2 - D_{JK}^v J(J+1)K^2 - D_K^v K^4 \quad (1.17)$$

where the D are centrifugal distortion constants and are very small compared to A and B (Herzberg, G., Infrared and Raman Spectra of Polyatomic Molecules, p. 26, Van Nostrand Reinhold Company, NY, 1945).

Equation 1.17 assumes that the rotational energy is non-degenerate. One then must add the vibration energy to equation 1.17 to get the total vibration-rotation energy of the molecule. The ν_7 vibration-rotation band of methyl cyanide has degenerate upper states due to a Coriolis interaction, however, and equation 1.17 must have additional correction terms added. A simple approximation for the energy becomes from Allen and Cross (Allen, H. and P. Cross, Molecular Vib-Rotors, p. 151, Wiley and Sons, Inc., New York, 1963)

$$\begin{aligned} \nu^Q = \nu_0 &+ [A'_v(1 - 2\zeta^2) - B'_v] \pm 2 [A'_v(1 - \zeta^2) - B'_v]K + [(A'_v - B'_v) - (A''_v - B''_v)]K^2 \\ &+ (B'_v - B''_v)J(J+1) \end{aligned} \quad (1.18)$$

where ν_0 is the vibrational energy contribution to the transition frequency called a Q-branch transition.

Asymmetric Rotor

The asymmetric rotor is more difficult than the symmetric rotor but one can begin with the Hamiltonian for a rigid rotor (Allen and Cross, p. 9)

$$H = \frac{1}{2} \left[\frac{J_x^2}{I_x} + \frac{J_y^2}{I_y} + \frac{J_z^2}{I_z} \right] \quad (1.19)$$

which has the same form for both symmetric and asymmetric molecules. We have also that

$$I_x \neq I_y \neq I_z \quad (1.20)$$

where I_x , I_y , and I_z are the moments of inertia along the principal axes of rotation. The assignments of the axes to the moments of inertia axes can be made in six different ways and the inverses of the moments of inertia multiplied by $\frac{\hbar^2}{2}$ are designated by A, B, and C where $A > B > C$. The representations of the moments of inertia are shown in Table 1.1 (Allen and Cross, p.26).

Table 1.1

Moments of Inertia Representations

	I^r	I^l	II^r	II^l	III^r	I^l
x	B	C	C	A	A	B
y	C	B	A	C	B	A
z	A	A	B	B	C	C

For ethylene, the representation of I^r is used. Now the Hamiltonian matrix given in equation 1.21 can be calculated.

$$H = \frac{1}{\hbar^2} [AJ_z^2 + BJ_x^2 + CJ_y^2] \quad (1.21)$$

A few relations are useful in the calculation of the matrix elements (Ewing, Alan, Masters thesis, University of Tennessee, p.10, 1993).

$$\langle j, k | J^2 | j, k \rangle = j(j+1)\hbar^2 \quad (1.22)$$

$$\langle j, k | J_z^2 | j, k \rangle = k^2\hbar^2 \quad (1.23)$$

$$\langle j, k | J_+^2 | j, k+2 \rangle = \{[j(j+1) - (k-1)(k-2)][j(j+1) - k(k-1)]\}^{\frac{1}{2}}\hbar^2 \quad (1.24)$$

$$\langle j, k | J_-^2 | j, k-2 \rangle = \{[j(j+1) - (k+1)(k+2)][j(j+1) - k(k+1)]\}^{\frac{1}{2}}\hbar^2 \quad (1.25)$$

It is also advantageous to use relations for the raising and lowering operators instead of J_x and J_y to solve the Hamiltonian matrix. Upon using those relations, the Hamiltonian becomes (Ewing, p.11)

$$H = \frac{1}{\hbar^2} \left[\left(\frac{B+C}{2} \right) J^2 + \left[A - \left(\frac{B+C}{2} \right) \right] J_z^2 + \left(\frac{B-C}{4} \right) (J_+^2 + J_-^2) \right] \quad (1.26)$$

and by utilizing the above equations, the non-zero matrix elements for the rigid rotor Hamiltonian

$$\langle j, k | H | j, k \rangle = \frac{B+C}{2} [j(j+1)] + \left[A - \left(\frac{B+C}{2} \right) \right] k^2 \quad (1.27)$$

$$\langle j, k | H | j, k+2 \rangle = \frac{B-C}{4} [(j-k)(j+k+1)(j-k-1)(j+k+2)]^{\frac{1}{2}} \quad (1.28)$$

$$\langle j, k | H | j, k-2 \rangle = \frac{B-C}{4} [(j+k)(j-k+1)(j+k-1)(j-k+2)]^{\frac{1}{2}} \quad (1.29)$$

The above expressions in conjunction with expressions for vibrational energies can give the energy levels of the transitions. Then using the selection rule for electric dipole transitions, the allowed transition frequencies can be determined. More advanced and complete theory and results are found in Gordy and Cook (Gordy, Walter and Robert L. Cook, Microwave Molecular Spectroscopy, Interscience Publishers,

New York, 1970) and Kroto (Kroto, H. W., **Molecular Rotation Spectra**, John Wiley & Sons, New York, 1975). The theory is necessary to this effort but beyond the scope of this review.

Chapter 2

Experimental Setup

Overview

This study involved the use of methyl cyanide data from the Fourier Transform Spectrometer (FTS) at the McMath Solar Telescope at Kitt Peak National Observatory (KPNO). These data were supplied by John J. Hillman of Goddard Space Flight Center (GSFC). Additional data were obtained in the Molecular Spectroscopy Laboratory at the University of Tennessee Department of Physics using the laboratory's tunable diode laser (TDL) spectrometer.

UTMSL Tunable Diode Laser Spectrometer

The instrument used for data acquisition is the tunable diode laser spectrometer. The TDL is an ideal spectrometer for obtaining line intensity measurements. The spectrometer produces high signal to noise ratio, narrow laser line widths enabling high spectral resolution, and depending on the diode being used, a fairly wide range of wavelengths can be tuned. The TDL laser chamber contains four diodes that are cryo-cooled by a CTI Cryogenics Helium Compressor. The detector used was a Hg-Cd-Te detector.

The laser head assembly operates in the 10-100K range. However TDL system evacuation is accomplished while the detector and TDL chamber are normally at room temperature. The pumping system consists of a liquid nitrogen cooled sorption pump and a large capacity ion pump. The sorption pump works because of a process known as physical adsorption. When a gas or molecule comes into contact with a solid or liquid surface, it physically attaches or adsorbs to the surface and is captured. Since the thickness of the film is only a few molecules thick, there must be a large surface area to give the

sorption pump a large capacity to be useful. A molecular sieve, a synthetic zeolite, gives a sorption pump a large capacity. It is highly porous with pore sizes just larger than the gas molecules so it has high surface area to volume ratio. Typically, there are more than 300 acres of surface area. When the material is cooled to liquid nitrogen temperature, the gas molecules are quickly adsorbed to the zeolite pores. This cooling produces a low pressure area inside the pump which allows material to flow from a high temperature, high pressure area to the sorption pump. When the pump warms, the gas desorbs from the surface and is released through a pressure relief valve. After several days of operation the sorption pump is heated to bake off the material drawn from the system. This insures that the pump is able to work at peak efficiency.

The other pump in the system is the ion pump. The ion pump is connected to a high voltage power supply capable of outputting 5000 volts. The ion pump cannot be used until the system has already been pumped down to a fairly low pressure. By understanding how the pump works, the previous statement becomes clearer. The ion pump consists of a center egg carton shaped metal chamber. On both sides of the chamber are titanium plates. The molecule or atom moves between the plates and is ionized by the high voltage and then migrates to the sides where it is captured by the titanium plate. This evacuates the chamber producing a low pressure area and thus causing a flow to the chamber. The ions pulled to the side are actually coated by metal. If there are too many molecules or atoms between the egg carton chamber and the plates, the power supply becomes overloaded (by design) and is unable to ionize the particles.

In addition to the main pumping system, the detector and the TDL chamber are outfitted with small ion pumps that continuously pump the chamber. This reduces the need for periodic pumping with the main system. The pumping system more than adequately achieves the minimum pressure of 50 milliTorr (while the TDL chamber is warm) for operation of the TDL when it is cooled to the 10-100K region.

In order to fill sample cells, a manifold system is used. It consists of a fore pump, diffusion pump and cold trap. The manifold system is connected to two pressure heads, a one Torr head and a 1000 Torr head. Only one is used at a time and is connected to a Baratron pressure gauge. The pressure gauges are absolute pressure gauges and are capacitance manometers. A small strip of flexible metal separates two chambers. If the pressure in the two chambers differs, the strip flexes and the capacitance changes. In an absolute pressure gauge, one side is evacuated to a known reference pressure and sealed at the factory. The other side is connected to the experimental chamber. The gauge measures the difference between the chamber pressure and the reference pressure. In a differential pressure gauge the two sides are connected to two different experimental chambers. The gauge measures the difference between the pressures in chamber one and chamber two. The pressure gauge also has output voltage jacks to connect to a voltmeter to monitor the pressure. This is the preferred setup. Currently a Beckman digital voltmeter monitors the voltage and allows a more accurate reading compared to the analog meter movement of the Baratron gauge. A Macleod gauge has been added to the manifold system to allow the measurement of absolute pressures. A diagram of the manifold system is shown in Figure 2.1. The manifold system is capable of pumping down to pressures of less than two milliTorr.

Changes have been made to the optics of the TDL spectrometer in order to perform the measurements on methyl cyanide. The previous optical setup is shown in Figure 2.2. This setup has most recently been used to determine the strength of absorption lines of ethylene by Alan Ewing (Ewing, Alan, Masters thesis, University of Tennessee, 1993) and to make acetylene line strength measurements by Dr. Mark Weber (Weber, Mark, Ph.D. dissertation, University of Tennessee, 1992) formerly of UTMSL and now of Goddard Space Flight Center. However, the largest sample cell that can easily be used has an absorbing path of 48.26 centimeters. For molecules with small dipole moments or for those with no dipole moments, this is more than adequate. But methyl cyanide has a very large dipole moment and therefore

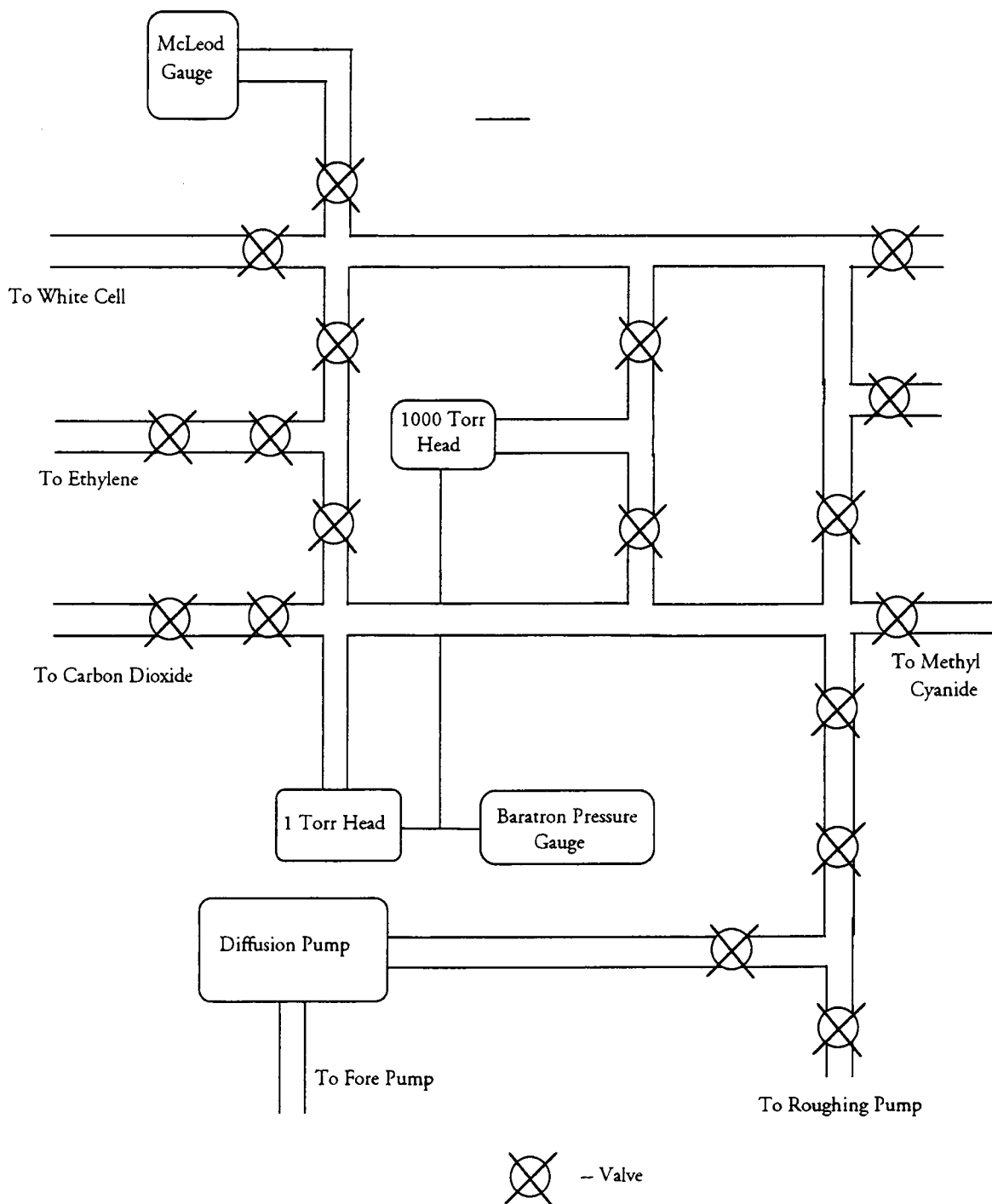


Figure 2.1

TDL Manifold Pumping System

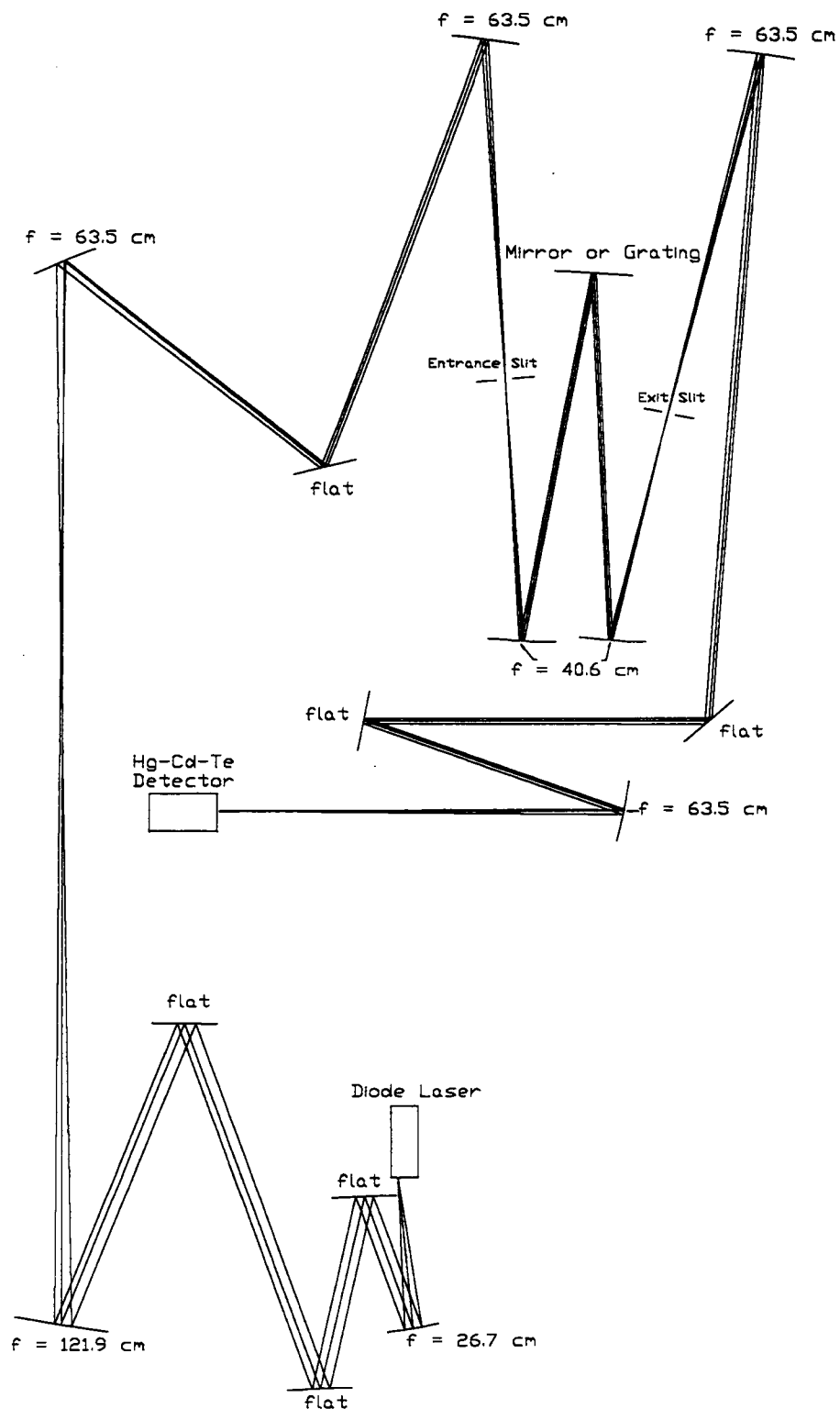


Figure 2.2

Main TDL Optical Diagram

requires long path lengths at low pressures to keep from seeing the effects of pressure broadening. Attempts were made to perform the experiment using the 48.26 centimeter cell but broadening was always present at even the lowest pressures that could be used to still see absorption lines. In order to give long path lengths for the sample, a White cell was integrated into the optics of the TDL system. The White cell, designed by Jennings (Jennings, D. E., W. E. Blass, and N. M. Gailar, *Absorption cell: a modified multiple-traversal device*, **Applied Optics**, Vol. 15, No. 4, p. 864, 1976) was previously used in the 5 meter Littrow spectrometer at UTMSL. Since it had been attached to the side of the 5-m spectrometer, a stand was built and the cell was placed on another table. The cell has a base path of 4 meters and by adjusting only one of the mirrors of the White cell, paths in multiples of 4 meters can be used. Previous use had indicated that the cell was not leak proof. In part this could be due to the O-rings used in the assembly of the cell. The cell was cleaned with ethanol and then heated and pumped to a low pressure. Once the cell was pumped down as low as it would go, a pressure increase test was performed. This enables one to determine if there is a leak or if there could be outgassing occurring. Figure 2.3 shows the pressure in the White cell versus elapsed time. The data indicated that the cell was leaking at a rate of about 1.7 milliTorr per hour. It was determined that this leak rate was tolerable for a 210 liter volume cell since it would be possible for this study to compensate for the leak rate.

Figure 2.4 shows the optical diagram for the new TDL system. The optics were designed to allow the use of just the main table, no White cell, by simply taking out two mirrors from the optical path. The optical design consists of a spherical mirror of focal length 26.7 cm that takes the energy from the diode and collimates it. Three flat mirrors then direct the beam to a 121.9 cm focal length mirror. After this mirror the beam passes through a sample cell and a 100 Hz chopper at the focal point. The beam is collected once again by a 63.5 cm mirror and is collimated once again. After this mirror is the position at which a germanium etalon can be inserted into the path to enable the calibration of the wavenumber scale using

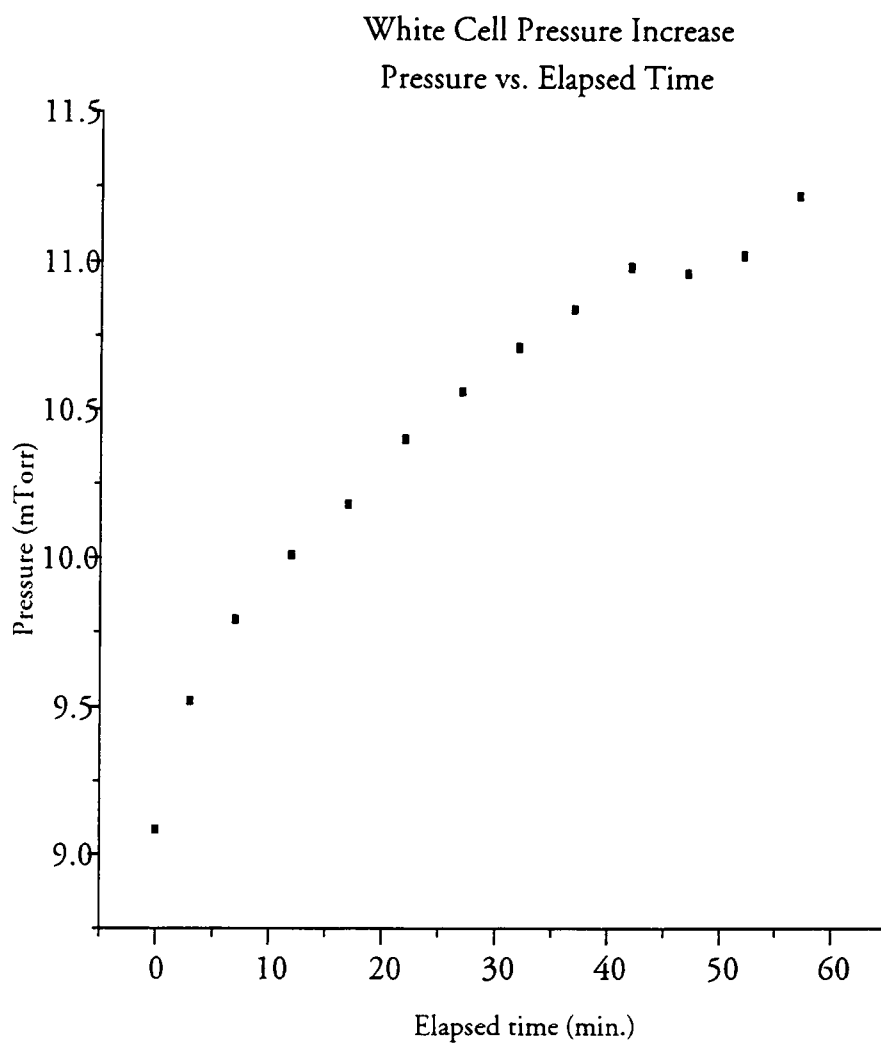


Figure 2.3.

White cell pressure increase curve

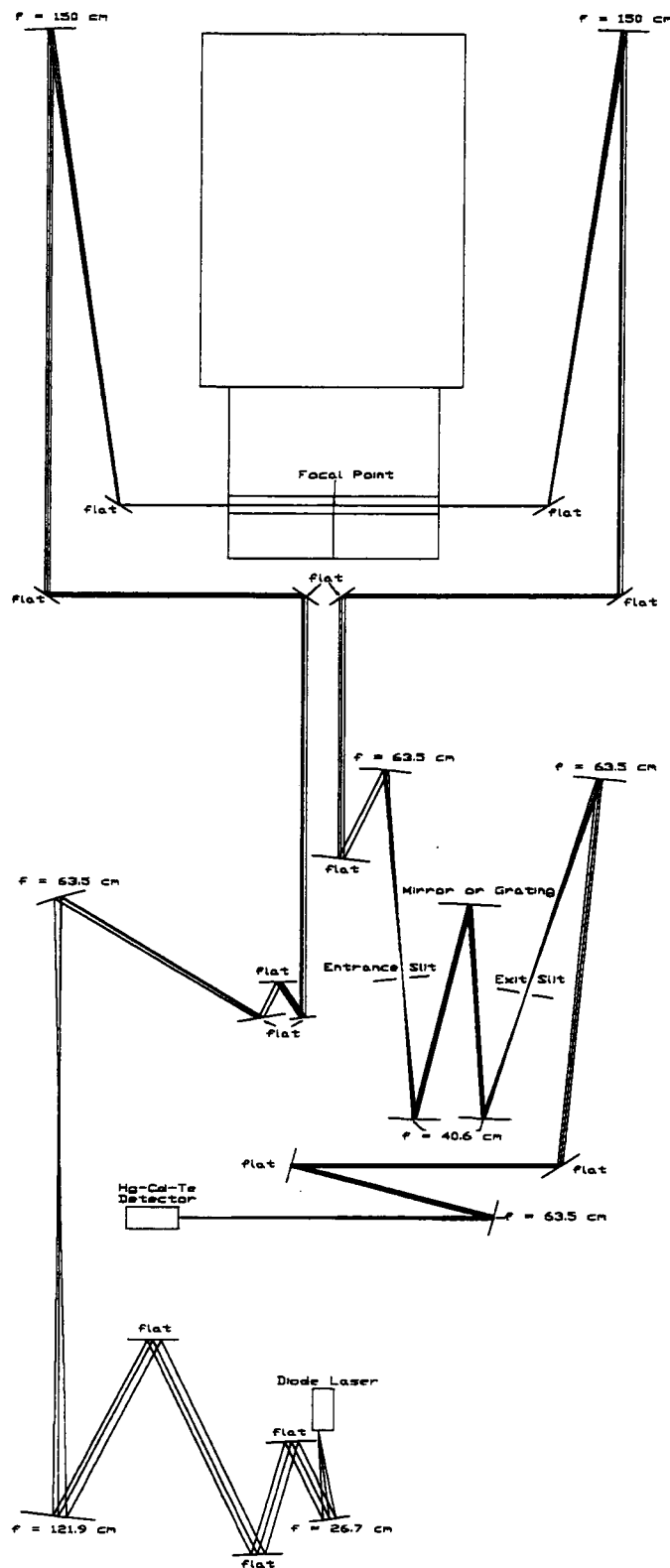


Figure 2.4
TDL Optical Diagram with White Cell

the fringes produced. The etalon has a fringe spacing of approximately 16 milliwavenumbers. The beam is then directed to a flat mirror. The next flat mirror has been added to the original design to send the beam to the White cell, located on another table. After picking off the beam, the next three flat mirrors direct the beam to a 150 cm focal length mirror located on the White cell table. This mirror focuses the beam to pass through the potassium bromide windows of the White cell. The beam comes to a focal point at the front edge of the inverted T shaped White cell mirror after being directed by an internal flat mirror just inside the White cell. The beam is then collected by a 50 cm focal length mirror that sends the beam to the 50 cm focal length White cell mirror. Depending upon the number of passes desired, the beam is directed to one or the other of the end 50 cm focal length mirrors before it is sent to the exit window of the White cell. An optical path diagram for the White cell is shown in Figure 2.5 with a four meter path length. Figure 2.6 shows the relative positions of the beams that strike the inverted T shaped mirror in the White cell for the eight meter path used in the experiment. The beam is then reflected off another 150 cm focal length mirror, collimating it before returning the main TDL table through a series of three flat mirrors. Once back on the main table, the beam is reflected off a 63.5 cm focal length mirror which brings the beam to a focus at the entrance slit. A 40.6 cm focal length mirror collimates the beam before it strikes the grating of the monochromator, or mirror, if doing optical alignment. Another 40.6 cm focal length mirror focuses the beam to pass through the exit slit of the system. A 63.5 cm focal length mirror collimates the beam once again and it is then sent toward the detector by two flat mirrors. It is brought to a focus on the detector by a 63.5 cm focal length mirror.

The alignment of the optical path is important for the success of our measurements. This is done by using a 3 mW Helium-Neon (He-Ne) laser. The He-Ne simplifies optical alignment by producing visible points of light on the mirrors. By the use of a pellicle and beam splitter, the He-Ne test beam is directed back to the diode laser and forward through the system. In addition, a beam is sent backwards through the system. This is done by sliding the detector to one side and allowing the backward beam to pass through a

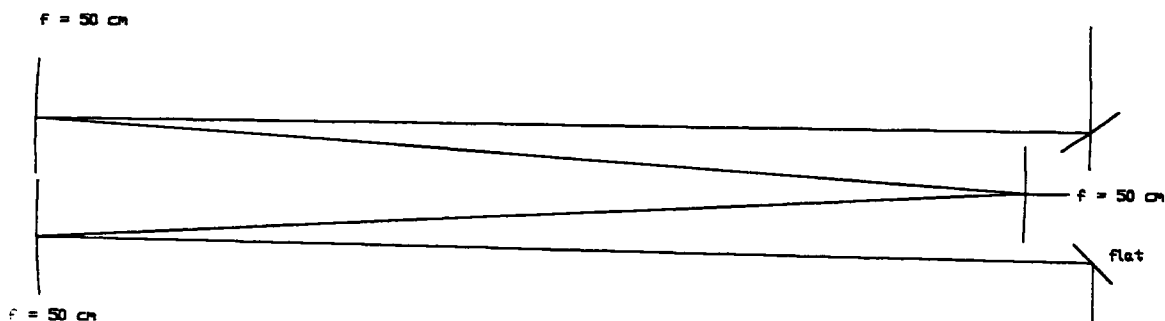


Figure 2.5

White cell optical path, 4 m path shown.

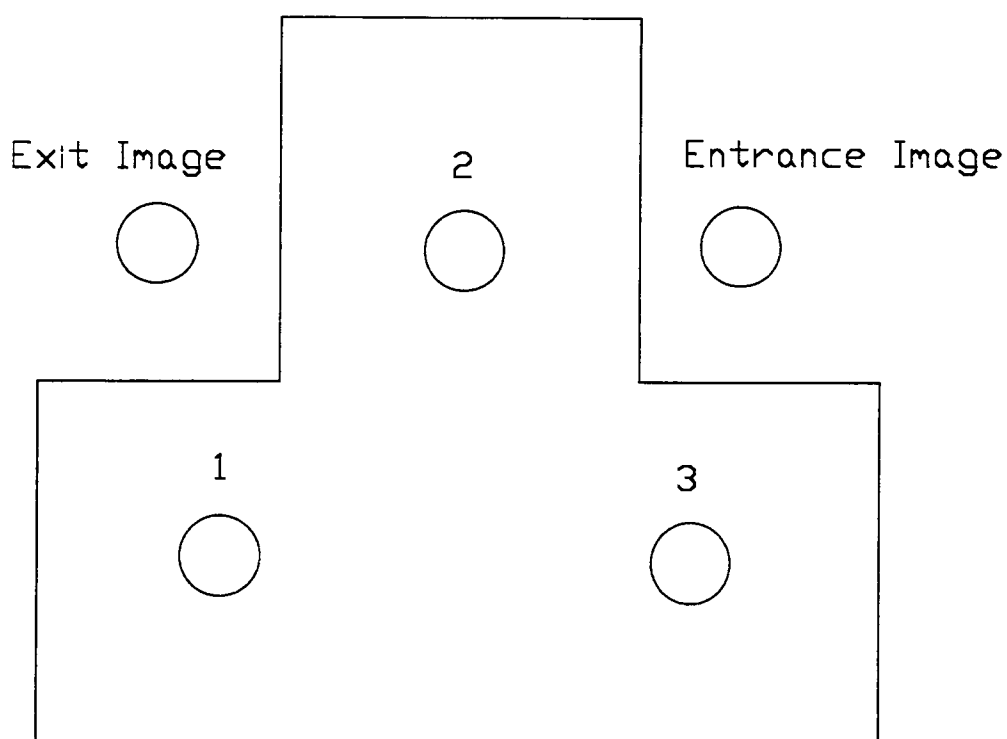


Figure 2.6

Positions of images on White cell mirror for 8 m path length

slit positioned at the previous detector position and then travel through the system. By positioning the forward and backward beams directly on top of each other on each mirror, the system can be brought to perfect optical alignment. This yields a maximum transmission of energy throughout the system. The only change to the optics is the replacement of the grating with a flat mirror.

Calibration of the grating is accomplished by using the He-Ne laser and the beam splitter. The grating will produce different order images of the test laser. The frequency of each order can be determined through the use of the grating equation

$$\nu_n = \frac{1}{\lambda n} \left(\frac{10^8 \text{ \AA}}{\text{cm}} \right) \quad (2.1)$$

where n is the order number and λ is the frequency of the He-Ne test laser (6328 Å). The calibration is begun by positioning the grating to direct the zero order beam on the exit slit. The zero order or central maximum can be easily found by using a white light source such as a flash light by shining the light through the entrance slit and observing the pattern produced on the exit slit. The central maximum will be a white light spot while higher orders will appear as their spectral components. Adjusting the grating to allow the central maximum to hit the exit slit, zeros the grating position. Now by using the He-Ne test laser, the grating can be rotated until the next order falls on the exit slit. The stepper motor position is recorded and then rotated to the next order. Once the grating stepper motor positions have been determined, the values are placed in a file to be used by the program SC149D written by the author and primarily, Alan Ewing. The program uses a bicubic spline to interpolate the wavenumber from the stepper motor position. SC149D is a Microsoft Windows program written in Visual Basic for Windows 2.0. The program allows the user to adjust stepper motor speed and direction by the use of a mouse. In addition, the program can send commands to the signal averager to start and stop scanning. A sample

calibration table listing the first ten orders is shown in Table 2.1. Normally, thirty orders are used in the calibration.

Table 2.1
Grating Calibration Data

Order #	ν (cm ⁻¹)	Step #
1	15802.8	867
2	7901.4	1710
3	5267.6	2558
4	3950.7	3406
5	3160.6	4265
6	2633.8	5131
7	2257.5	5967
8	1580.3	8565
9	1436.6	9449
10	1316.9	10317

Calibration of the line widths of the data is accomplished by using the germanium etalon. The spacing between fringes can be calculated using the equation

$$\Delta \nu = \left[\frac{1}{2nl} \left(1 - \frac{\lambda}{n} \frac{\partial n}{\partial \lambda} \right) \right] \quad (2.2)$$

where n is the refractive index of the etalon ($n = 4$ for the UTMSL etalon) and l is the cavity length and λ is the wavelength of light. An etalon scan is taken after each data scan to calibrate the spacing between channel numbers of the signal averager. A wide etalon scan is taken and overlapped with a wide data scan to determine exact etalon fringe spacing by using Kitt Peak data and known line positions. The spacing for the UTMSL etalon is 16.023 milliwavenumbers.

Temperature of the sample gas must be measured accurately in order to determine Doppler widths and to adjust intensity measurements to standard temperature. The temperature is measured using a thermocouple connected to an Omega Engineering DP41- TC High Performance Temperature Indicator. The thermocouple is iron-constantan. The temperature is read from the LED display in Kelvin, accurate to 0.1 K. The thermocouple is easily attached and removed by use of tape on the sample cell.

Experimental Procedure

Now that the equipment for measuring spectra has been described, the experimental procedure can be explained. In order to achieve optimum results the following procedure was followed. The laser diode temperature was allowed to stabilize for approximately 20 or 30 minutes before any data were taken. The sample cell, in this case the White cell, was filled to the desired pressure and was allowed to equilibrate for at least 20 minutes. This was normally done while allowing the laser to come to operating

temperature initially. The Krohn-Hite signal generator was turned on, enabling the chopper to run and to trigger both the oscilloscope and the signal averager. The laser was then turned on and the grating was turned to allow the energy to pass to the detector.

An actual data scan is done by following the procedure below.

1. Adjust current to the laser diode to the desired location in the spectra.
2. Rotate the grating to achieve maximum energy to the detector.
3. Select Normal Averaging mode on Signal Averager and set the number of scans. Typically the number of scans is between 5 and 500. Perform data scan.
4. Using the Terminal program from Microsoft Windows, download data into file to be analyzed.
5. Place etalon in optical path. Repeat steps 3 and 4.
6. Perform wide data scan by adjusting Krohn-Hite ramp voltage and repeat steps 3, 4 and 5. This can be used to calibrate the etalon fringe spacing.
7. The data is analyzed using the program N17 written by Mark Weber. The program uses the etalon scan to calibrate wavenumbers per data point. The data is then read into the program and the user sets the baseline and zero transmission of the spectral line before the program performs a fit to determine the equivalent width, half width at half maximum (HWHM), and the line transmission value (τ).

One problem that arises in a TDL system is the inability to determine exact line positions in the spectra.

One usually knows the region but since methyl cyanide has spectral lines that are virtually duplicated from one wavenumber to the next, exact determination of lines proved to be difficult. In order to facilitate this, a 48.26 cm cell filled with ethylene was placed in the optical path. An etalon scan can be overlapped as well, and knowing that the spacing of the etalon is 16.023 milliwavenumbers, distances between spectral lines can be determined and then compared with a list of lines for that region. Figure 2.7 shows a typical scan with methyl cyanide only, methyl cyanide and ethylene lines present, and a

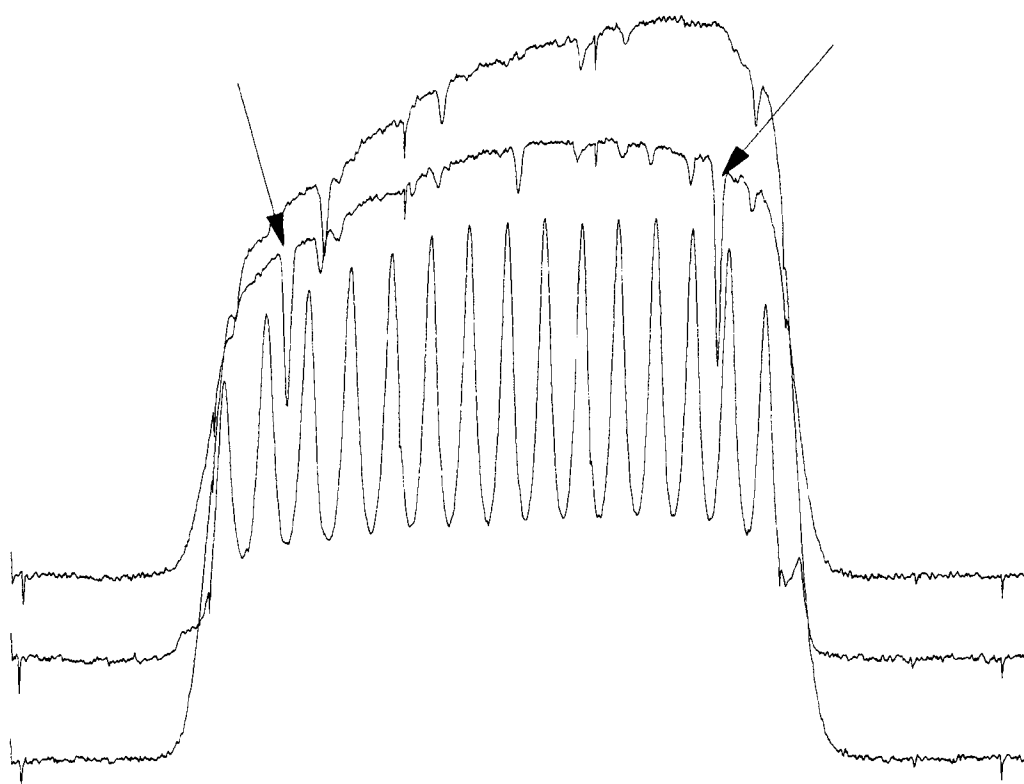


Figure 2.7

Wide TDL scans with top scan showing CH₃CN only, middle scan showing CH₃CN and C₂H₄, and corresponding etalon scan on bottom. The two arrows point to two strong C₂H₄ lines.

corresponding etalon scan. Figure 2.8 shows a narrow scan used by N17 with a corresponding etalon scan overlapped.

Recent Experimental Design Change

A puzzling problem had been noticed with the TDL system. Absorption lines were being broadened to the point that Doppler width lines were not achievable. The absorption lines when viewed with an oscilloscope or the signal averager appeared to be visible at two distinct positions. Each line appeared to oscillate between the two positions and because of this, the signal averager averaged the two apparent lines creating an absorption line with a much greater than Doppler half width at half maximum.

The problem was attributed to a vibration problem and led to a design change. The TDL system originally had the laser mounted to the same table as the detector and all of the optics. The cold head of the laser was believed to be causing a vibration of the aluminum table, causing the table to act as a drum head. A mount constructed from a 55 gallon barrel filled with sand and a concrete pillar resting on top of the sand was built. A small aluminum table was fastened the concrete pillar and the diode laser was mounted on the table. The sand, it was believed, would help to dampen vibrations from the building and the laser would not vibrate any optics or the detector since it was isolated from the main table. An optical diagram of the new design without the White cell in the path is shown in Figure 2.9.

At first the design change appeared to make no difference in the data. The lines were still being broadened but for no apparent vibrational problem. The current ramp from the signal generator to the laser diode current controller was tested next and was found to have a large amount of noise. This noise was causing the laser diode to scan forward and backward in wavelength as the ramp increased. This caused the signal averager to average multiple line positions. This problem was found to be caused by a

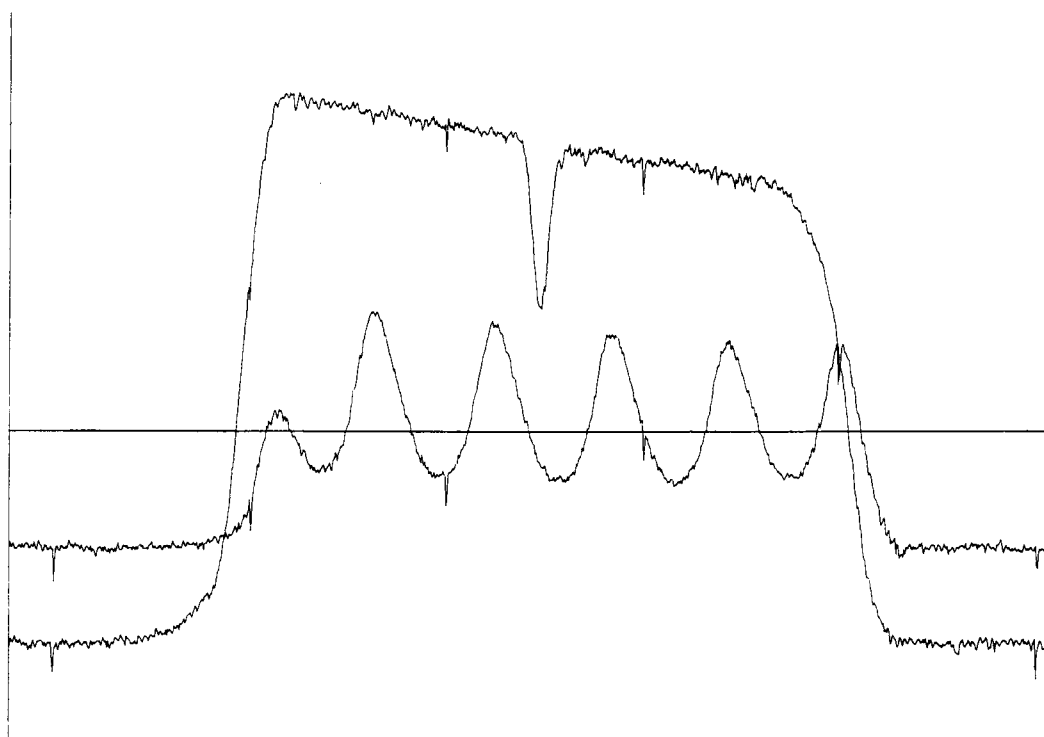


Figure 2.8

Narrow TDL scan of C_2H_4 with etalon scan overlapped.

C_2H_4 line is at $951.73787 \text{ cm}^{-1}$.

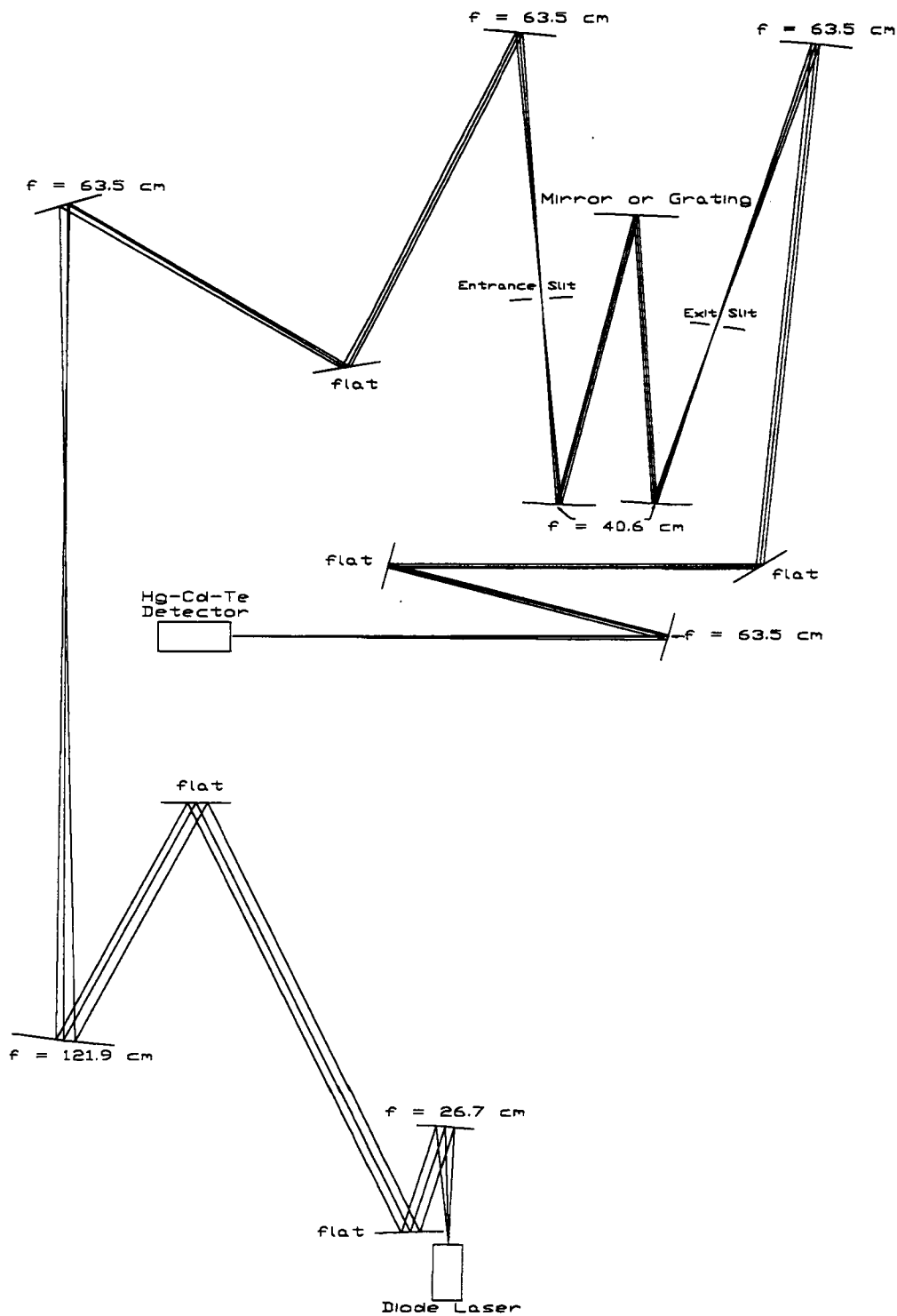


Figure 2.9

New optical design of TDL system.

ground loop and was quickly repaired by grounding all equipment to the same point. The subsequent data proved to be much improved and the half widths at half maximum of the absorption lines were very close to Doppler. It was then possible to repeat the ethylene experiment in about two weeks which had taken several months before the design change. There was no time to repeat the methyl cyanide portion of the experiment however.

Chapter 3

Experimental Results

Overview

Experimental data for methyl cyanide were obtained from Kitt Peak National Observatory (KPNO) and also University of Tennessee Molecular Spectroscopy Laboratory (UTMSL). The Kitt Peak data were used to make transition energy assignments. The transitions are between ground rotational states and upper vibration-rotation energy states. Data were obtained from the $2\nu_8$, ν_4 , ν_7 , and $3\nu_8$ vibration-rotation bands ranging from about 600 cm^{-1} to about 1125 cm^{-1} . UTMSL data were used for intensity measurements. Absorption line intensities were measured in the ν_4 (949 cm^{-1}) region and also the ν_7 (1041 cm^{-1} - 1100 cm^{-1}) region.

In addition to the methyl cyanide UTMSL data, ethylene (C_2H_4) absorption data were also obtained for intensity measurements. The absorption lines were in the 940 cm^{-1} to 970 cm^{-1} region. FTS data from KPNO were also used for intensity measurements. Alan Ewing of UTMSL reported many intensity measurements from both KPNO and UTMSL data in his Master's thesis (Ewing, Alan, Masters thesis, 1993).

FTS Data, Transition Assignments

Analysis of the methyl cyanide spectra was accomplished using DECOMP, an FTS spectral decomposition program (Abrams, Mark, Ph.D. dissertation, University of California, Berkley, 1990) and various methods to be described in the following discussion. DECOMP provides a graphical user interface to analyze spectra taken at the Kitt Peak National Observatory. DECOMP enables the user to quickly determine line

positions and can also aid in the determination of line strengths. A sample screen from DECOMP is shown in Figure 3.1. The R side of the ν_7 band will be the emphasis of discussion.

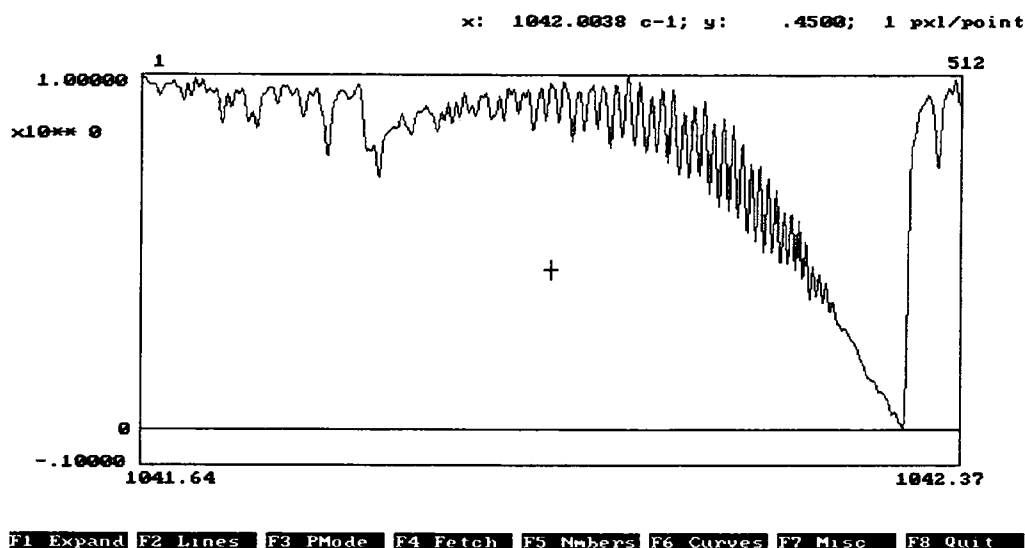


Figure 3.1

Sample DECOMP screen showing the R_{Q_0} branch of CH_3CN

The ν_7 band of methyl cyanide is a perpendicular band. A perpendicular band has the selection rules of $\Delta K = \pm 1$, $\Delta J = 0, \pm 1$ while a parallel band, such as the ν_4 and $2\nu_8$ bands, has selection rules of $\Delta K = 0$, $\Delta J = 0, \pm 1$. The assignment notation to be used here follows the standard convention of

$$\Delta K \Delta J_K(J) \quad (3.1)$$

Transitions for the perpendicular band also must not have $J < K$. For example, the transition $R_{R_3(2)}$ is a forbidden transition.

Method of Analysis

The first part of the assignments of the ν_7 band was made on a spectral plot. The Kitt Peak National Observatory (KPNO) data was plotted using a Nicolet plotter. The plotting program, written by Dr. Mark Weber, formerly of UTMSL, allows the user to specify plotting ranges in wavenumbers and a scale corresponding to wavenumbers/inch. For the first assignments, the energy equation for transitions from ground state can be approximated as

$$\nu(J,K) = \nu_0 + 2B_0J(J+1) \quad (3.2)$$

where ν_0 is the sub-band origin and B_0 is a ground state rotational constant.

The value of B_0 is well known. Rackley et. al. (Rackley, S. A., R. J. Butcher, M. Römheld, S. M. Freund, and T. Oka, *Laser Stark Spectroscopy of Methyl Cyanide in the 10- μ m Region: Analysis of the ν_4 and ν_7 Bands, and the ν_7 , $3\nu_8^1$ Interaction*, **Journal of Molecular Spectroscopy**, **92**, p. 203—217, 1982.)

reported that the constant has a value of $0.306842252(3) \text{ cm}^{-1}$. This gives the spacing between transition lines to be about 0.6 cm^{-1} . It is possible then to assign transitions on the spectral plots looking for lines that are separated by about 0.6 cm^{-1} and then to follow the series of lines back to a sub-band origin, ν_0 in equation 3.2.

DECOMP was used to determine the exact line positions. DECOMP's LINELIST function was used to determine the peak location of a transition line using a 2 point gaussian and first derivative test. The data generated were used in conjunction with assigned spectral plots to determine the transition energy of the lines.

Calibration of Methyl Cyanide Energies

The data received from KPNO was found to have ethylene (C_2H_4) lines present. These proved to be valuable in determining a frequency calibration for the methyl cyanide lines. Table 3.1 shows the ethylene lines found in the CH_3CN spectra and the reference known positions of the ethylene lines. The known lines were obtained from KPNO ethylene spectra being analyzed by UTMSL. The ethylene lines in the C_2H_4 spectra were calibrated from very well known line positions of CO_2 . The ethylene calibration can be found in Alan Ewing's thesis (Ewing, p. 39) of UTMSL. The calibration factor for methyl cyanide data was obtained from the plot shown in Figure 3.2 and results in the following equation to determine calibrated line positions from the observed values:

$$\nu(\text{corr}) = (1.000004748)[\nu(\text{uncorr})]. \quad (3.3)$$

Ground State Combination Differences

The use of ground state combination differences (GSCD) (Blass, W. E., Ph.D. dissertation, Michigan State University, 1963) aids in the assignment of transitions and also provides a method for checking assignments already made. This proved to be very useful in the assignments of the Q branches of the ν_7 band.

Ground state energies for the ν_7 band were calculated using ground state constants from previous work in the far IR region. Values for the constants were obtained from Brown et. al. (Brown, F., D. Dangoisse, and J. Demaison, *The Rotational Spectrum of CH_3CN above 1000 GHz*, **Journal of Molecular Spectroscopy**, 129, 483-485, 1988) and Carlotti et. al. (Carlotti, Di Lonardo, Fusina, and Carli, *The Far-*

Table 3.1

Ethylene Absorption Line Energies in Wavenumbers from
 Calibrated KPNO Ethylene Spectra and uncalibrated (observed) KPNO Methyl Cyanide Spectra

C ₂ H ₄ Line Positions (C ₂ H ₄ Spectra) (cm ⁻¹)	C ₂ H ₄ Line Positions (CH ₃ CN Spectra) (cm ⁻¹)
949.0061	949.00109
949.01475	949.0098
949.10735	949.1026
949.2004	949.19563
949.28795	949.2836
949.33506	949.33014
949.34173	949.3369
949.34735	949.34262
949.37255	949.36781
950.05629	950.0516
950.33116	950.32631
950.64985	950.64528
951.37166	951.36707
973.5524	973.5478
975.42112	975.4169
975.99622	975.9914
977.24512	977.2406
979.63273	979.6285
980.90593	980.9015
982.39173	982.3872
984.64184	984.6374
985.52304	985.5183
986.01064	986.0057
986.51454	986.5095
987.48644	987.4816
987.99104	987.9866
988.51514	988.5106
990.90475	990.9011
993.36805	993.3629
996.24445	996.2408
997.30746	997.3027
998.50986	998.5052

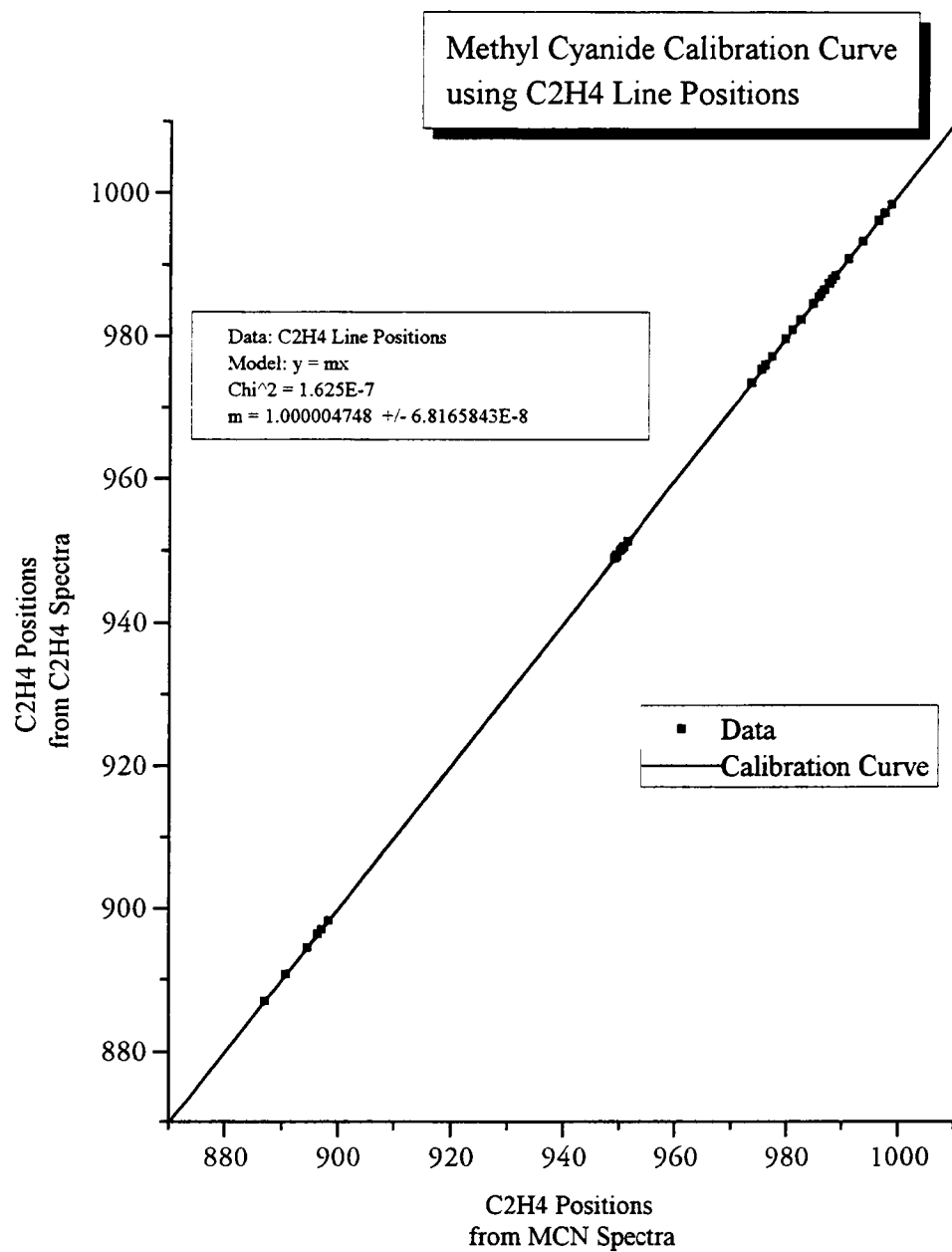


Figure 3.2

Methyl Cyanide Calibration Curve

for the ground vibrational state energy equation

$$E_{GS}(J, K) = BJ(J+1) + (A-B)K^2 - D_J[J(J+1)]^2 - D_{JK}J(J+1)K^2 - D_KK^4 + H_J[J(J+1)]^3 + H_{JK}[J(J+1)]^2K^2 + H_{KJ}J(J+1)K^4 + H_KK^6 + L_J[J(J+1)]^4 + L_{JK}[J(J+1)]^3K^2 + L_{JK}[J(J+1)]^2K^4 + L_{KKJ}J(J+1)K^6 + L_KK^8 \quad (3.4)$$

where D_J , D_{JK} , D_K , H_J , H_{JK} , H_{KJ} , H_K , L_J , L_{JK} , L_{JK} , L_{KKJ} , and L_K are centrifugal distortion terms. The values of these constants are given in Table 3.2.

Table 3.2

Molecular constants used to calculate ground state energies

Molecular Constant	Value (cm ⁻¹)
B_0	0.306629974
A_0	5.243333
D_J	0.000000126921
D_{JK}	0.000005912931
D_K	0.0000946666
H_J	$-8.10037666 \times 10^{-15}$
H_{JK}	$3.3877741 \times 10^{-11}$
H_{KJ}	$1.939678867 \times 10^{-10}$
H_K	0
L_J	0
L_{JK}	$-2.45276533 \times 10^{-7}$
L_{JK}	0
L_{KKJ}	3.414×10^{-5}
L_K	0

It is worth noting that the GSCD method of assignment will only work if the transitions are to the same upper state. For most transitions, related transitions do terminate on the same upper state. For the $K = 0$

sub-band of a perpendicular band the usually common upper state may be split by l doubling or a Coriolis resonance. In the ν_7 band of methyl cyanide this does occur. This type of energy level splitting occurs because the molecule can execute equivalent vibrations in either of two perpendicular planes. When this is coupled with a rotational motion, degeneracy in the energy state is removed because in one plane the Coriolis force slightly increases the energy and in the other plane the Coriolis force is zero (Allen, H. and P. Cross, Molecular Vib-Rotors, p. 51, Wiley and Sons, Inc., NY, 1963). Due to this energy level splitting, the ${}^RQ_0$ transitions terminate in a different upper energy state than do the related ${}^RR_0$ and ${}^RP_0$ transitions. This invalidates the use of GSCD's to determine the energies of the ${}^RQ_0$ transitions from readily assigned ${}^RR_0$ and ${}^RP_0$ transitions. However, once the energy spacing between l doubled and/or Coriolis split levels is known, the assignments can be made.

The equation used to predict line energies for a perpendicular band can be written as

$${}^R R_K(J) - [E(K, J+1) - E(K, J)] = {}^R Q_K(J+1) \quad (3.5)$$

for one type where the term in brackets is the ground state energy difference between two levels. Other formulae for calculating transition energies of ${}^RP_K$, ${}^P P_K$, etc. are very similar and work as long as the transitions are to the same upper state. The diagram in Figure 3.3 shows GSCD as a level scheme (Dakhil, M., Ph.D. thesis, University of Tennessee, 1983) and Figure 3.4 shows an example from the $3\nu_8^1$ band for calculating the ${}^RQ_6$ absorption lines.

Assignments of the ${}^RQ_0$ band were calculated through the use of GSCD and then verified for position on the spectral plot. Because of the l splitting, only an effective value for α_B could be obtained from plots of ${}^R R_0(J)$ transition energy versus m number where m is $J+1$ for R-side of the Q-branch and $-J$ for P-side of the branch. A plot of the R-side transition energy versus m number is shown in Figure 3.5.

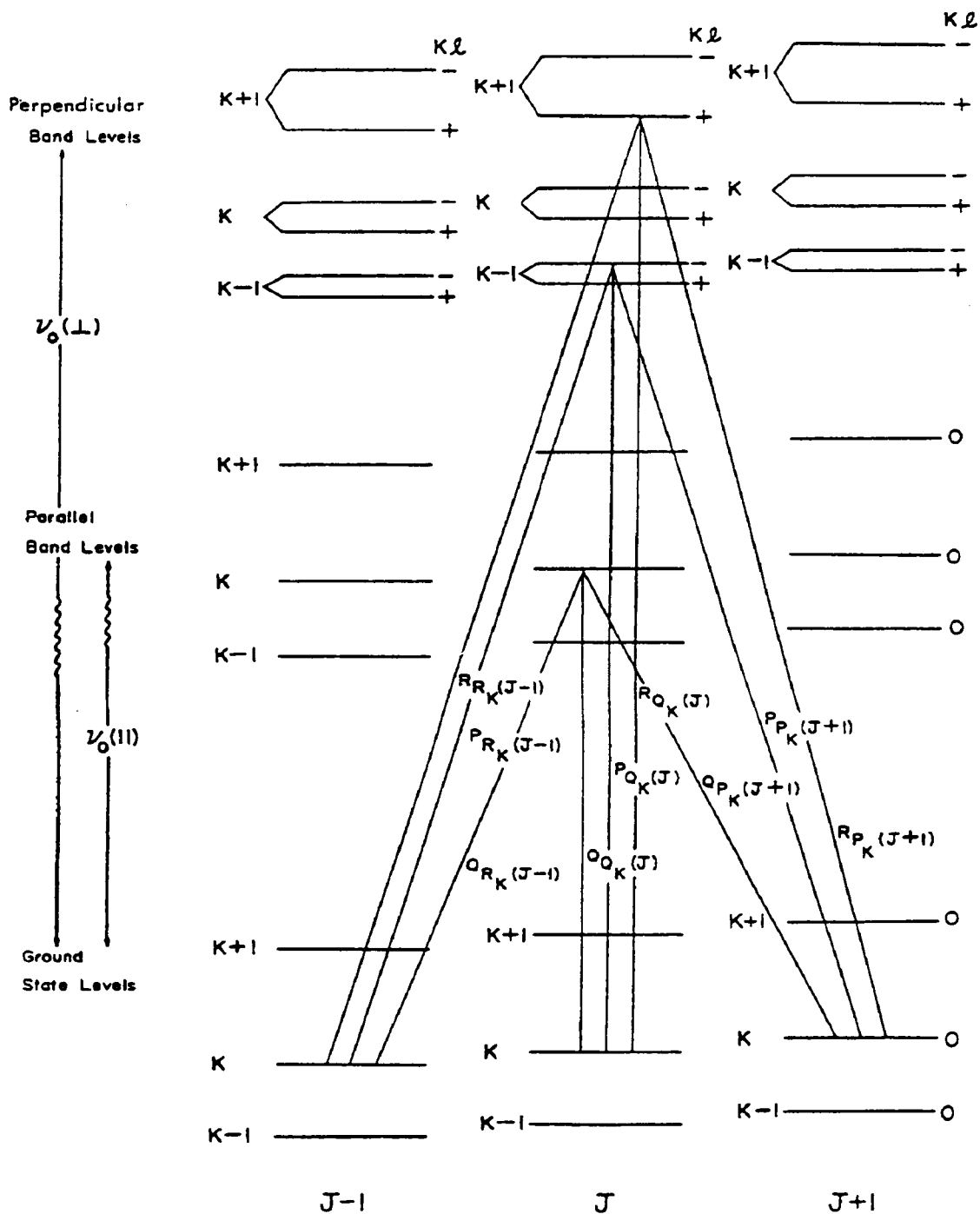
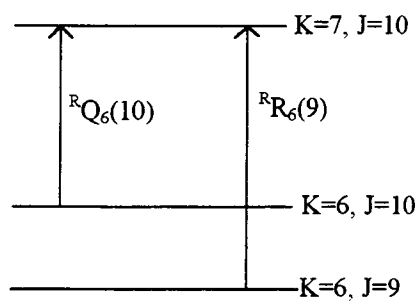


Figure 3.3

GSCD Level Scheme



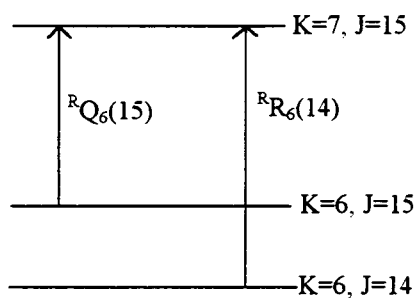
Ground State Energies: $E(6,10) = 211.449303600 \text{ cm}^{-1}$

$E(6,9) = 205.31721700 \text{ cm}^{-1}$

$${}^R R_6(9) = 1084.646 \text{ cm}^{-1}$$

$${}^R Q_6(10) = {}^R R_6(9) - [E(6,10) - E(6,9)]$$

$${}^R Q_6(10) = 1078.513913 \text{ cm}^{-1}$$



Ground State Energies: $E(6,15) = 251.3054136 \text{ cm}^{-1}$

$E(6,14) = 242.1082272 \text{ cm}^{-1}$

$${}^R R_6(14) = 1087.92847 \text{ cm}^{-1}$$

$${}^R Q_6(15) = {}^R R_6(14) - [E(6,15) - E(6,14)]$$

$${}^R Q_6(15) = 1078.731284 \text{ cm}^{-1}$$

Figure 3.4

Sample GSCD Calculations

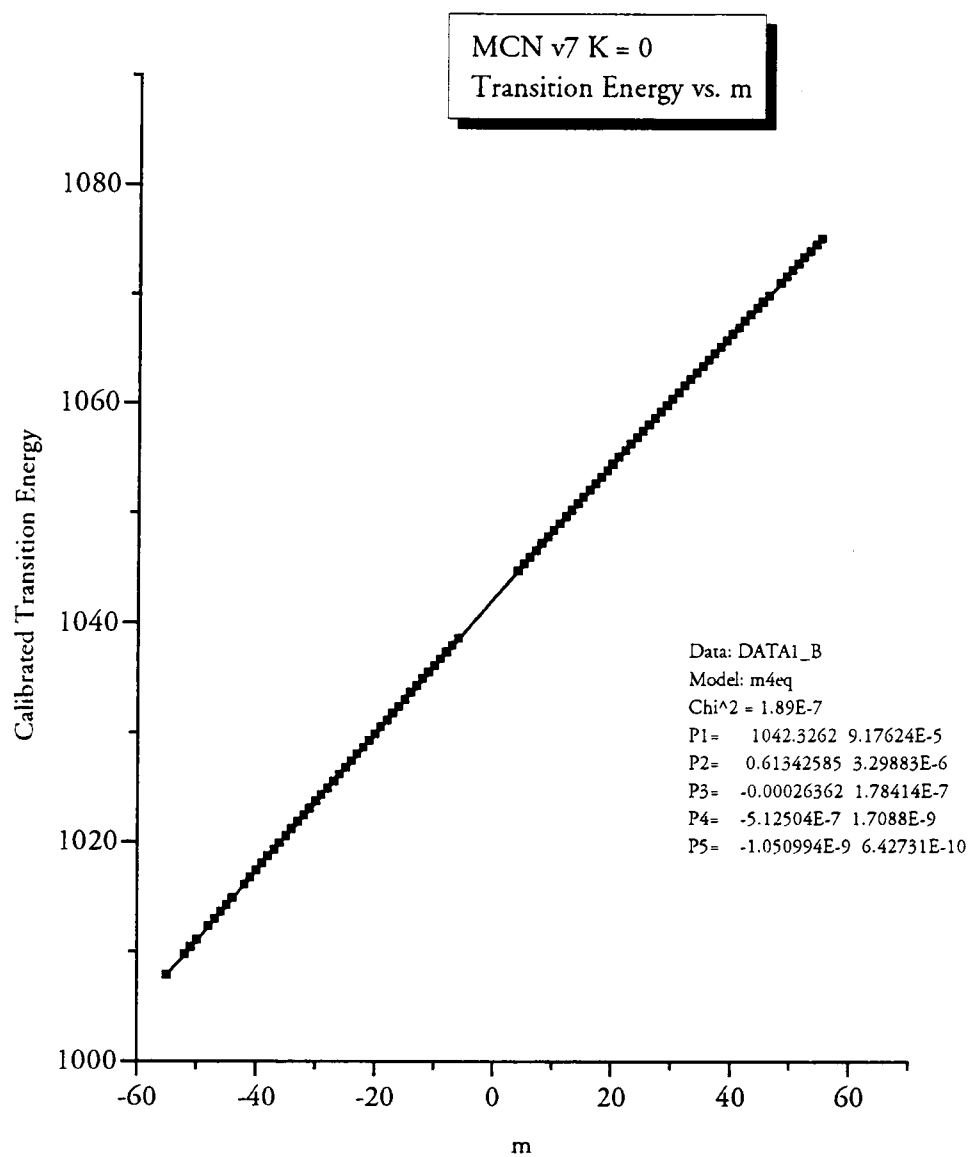


Figure 3.5

$^R R_0(J)$ transition energies vs m number graph

The data were fit to a fourth order polynomial and a value of 2.6362×10^{-4} was determined for an effective value of α_B . A value for α_B of 1.875×10^{-4} for the whole band, $K > 0$, was reported by Mori, et. al. (Mori, Y., T. Nakagawa, and K. Kuchitsu, *Vibration-Rotation Spectra of CH₃CN: The ν_7 Band and Its Hot Bands near 1040 cm^{-1}* , *Journal of Molecular Spectroscopy*, **104**, p.388-401, 1984) for the ν_7 band. By using the equation

$$\alpha_{B_{eff}} = \alpha_B - \frac{1}{2} q_7^{(+)} \quad (3.6)$$

where $q_7^{(+)}$ is the l -doubling constant term, a value of $1.1138 \times 10^{-4}\text{ cm}^{-1}$ was calculated for the effective value of α_B for ${}^RQ_0$ enabling one to use the equation

$$\nu_Q = \nu_0 - \alpha_{B_{eff}} J(J+1) \quad (3.7)$$

to calculate the energies of the branch. The assignments of the Q branch can be found in Table 3.3. The spacing in wavenumbers between J and $J+1$ of the ${}^RQ_0$ absorption lines was also used to determine the assignments and can also be found in Table 3.3.

Perturbations to the ${}^RQ_6$, ${}^RQ_7$, and ${}^RQ_8$ bands were apparent from spectral plots. The $3\nu_8^1$ band causes a Fermi resonance with ν_7 . Due to this resonance, the weak $3\nu_8^1$ band robs intensity from the ν_7 band and some lines from the ${}^RQ_6$ branch and ${}^RQ_8$ lines are visible. These lines are included in the table as well. The ${}^RQ_6$ lines were visible up to $J = 23$ and from these assignments the ${}^RQ_6$ lines were calculated using GSCD and then identified in the spectral plot. Some plots of the ${}^RQ_6$, ${}^RQ_7$, and ${}^RQ_8$ branches from the ν_7 band and the ${}^RQ_6$ and ${}^RQ_8$ lines of the $3\nu_8^1$ band are shown in Figure 3.6. Because of the perturbation caused by the $3\nu_8^1$ band, the ${}^RQ_6$ branch actually is backward as compared to ${}^RQ_5$ branch for instance and the ${}^RQ_6$ lines actually reverse direction at higher J values. As for the ${}^RQ_7$ branch, the ${}^RQ$ lines increase in

Table 3.3

Calculated and Observed ${}^RQ_0$ assignments in wavenumbers

j	Calculated Transition Energy of ${}^RQ_0(J)$ (cm^{-1})	Spacing between Calculated Energies ${}^RQ_0(J+1) - {}^RQ_0(J)$ (cm^{-1})	Measured Transition Energy of ${}^RQ_0(J)$ (cm^{-1})	Spacing between Observed Energies ${}^RQ_0(J+1) - {}^RQ_0(J)$ (cm^{-1})
0	1042.3262	-0.00022276		
1	1042.325977	-0.00044552		
2	1042.325532	-0.00066828		
3	1042.324863	-0.00089104		
4	1042.323972	-0.0011138		
5	1042.322859	-0.00133656		
6	1042.321522	-0.00155932		
7	1042.319963	-0.00178208		
8	1042.318181	-0.00200484		
9	1042.316176	-0.0022276		
10	1042.313948	-0.00245036		
11	1042.311498	-0.00267312		
12	1042.308825	-0.00289588		
13	1042.305929	-0.00311864		
14	1042.30281	-0.0033414		
15	1042.299469	-0.00356416		
16	1042.295905	-0.00378692		
17	1042.292118	-0.00400968		
18	1042.288108	-0.00423244		
19	1042.283876	-0.0044552		
20	1042.27942	-0.00467796		
21	1042.274742	-0.00490072		
22	1042.269842	-0.00512348		
23	1042.264718	-0.00534624		
24	1042.259372	-0.005569	1042.257989	-0.00634003
25	1042.253803	-0.00579176	1042.251649	-0.006000028
26	1042.248011	-0.00601452	1042.245649	-0.005820028
27	1042.241997	-0.00623728	1042.239829	-0.00641003
28	1042.235759	-0.00646004	1042.233419	-0.00638003
29	1042.229299	-0.0066828	1042.227038	-0.006730032
30	1042.222617	-0.00690556	1042.220308	-0.006700032
31	1042.215711	-0.00712832	1042.213608	-0.007410035
32	1042.208583	-0.00735108	1042.206198	-0.007240034
33	1042.201232	-0.00757384	1042.198958	-0.007580036
34	1042.193658	-0.0077966	1042.191378	-0.007650036
35	1042.185861	-0.00801936	1042.183728	-0.008200039

Table 3.3 (cont.)

Calculated and Observed ${}^RQ_0$ assignments in wavenumbers

j	Calculated Transition Energy of ${}^RQ_0(J)$ (cm^{-1})	Spacing between Calculated Energies ${}^RQ_0(J+1) - {}^RQ_0(J)$ (cm^{-1})	Measured Transition Energy of ${}^RQ_0(J)$ (cm^{-1})	Spacing between Observed Energies ${}^RQ_0(J+1) - {}^RQ_0(J)$ (cm^{-1})
36	1042.177842	-0.00824212	1042.175528	-0.008290039
37	1042.1696	-0.00846488	1042.167238	-0.008650041
38	1042.161135	-0.00868764	1042.158588	-0.008550041
39	1042.152447	-0.0089104	1042.150038	-0.008930042
40	1042.143537	-0.00913316	1042.141108	-0.009160043
41	1042.134404	-0.00935592	1042.131948	-0.009030043
42	1042.125048	-0.00957868	1042.122918	-0.010120048
43	1042.115469	-0.00980144	1042.112798	-0.009960047
44	1042.105668	-0.0100242	1042.102838	-0.009660046
45	1042.095643	-0.01024696	1042.093178	-0.01057005
46	1042.085396	-0.01046972	1042.082608	-0.010660051
47	1042.074927	-0.01069248	1042.071948	-0.010660051
48	1042.064234	-0.01091524	1042.061288	-0.011470054
49	1042.053319	-0.011138	1042.049818	-0.011740056
50	1042.042181	-0.01136076	1042.038078	-0.010900052
51	1042.03082	-0.01158352	1042.027178	-0.012280058
52	1042.019237	-0.01180628	1042.014897	
53	1042.00743	-0.01202904		
54	1041.995401	-0.0122518		
55	1041.98315	-0.01247456		
56	1041.970675	-0.01269732		
57	1041.957978	-0.01292008		
58	1041.945058	-0.01314284		
59	1041.931915	-0.0133656		
60	1041.918549			

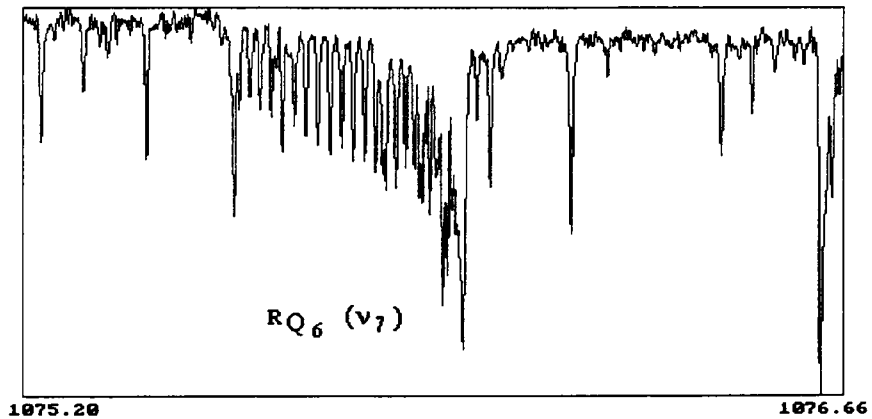
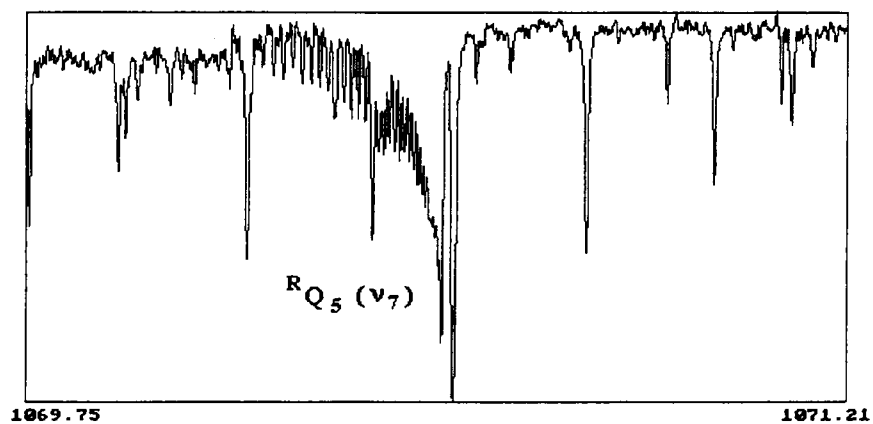


Figure 3.6

Example Q branches from CH_3CN spectrum

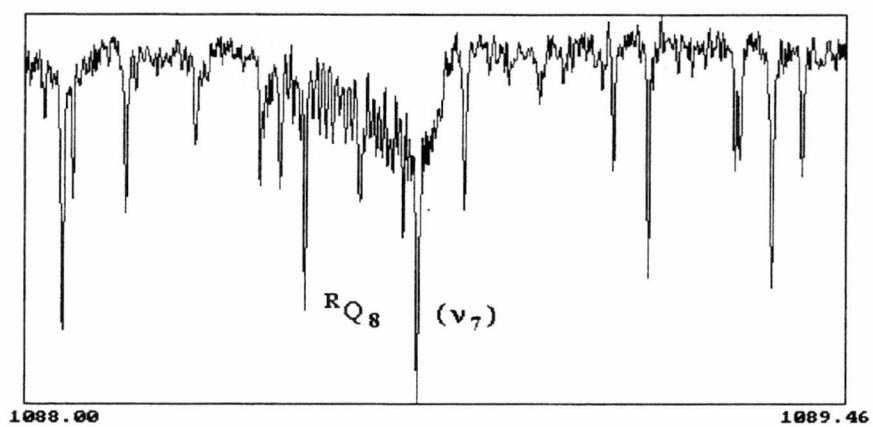
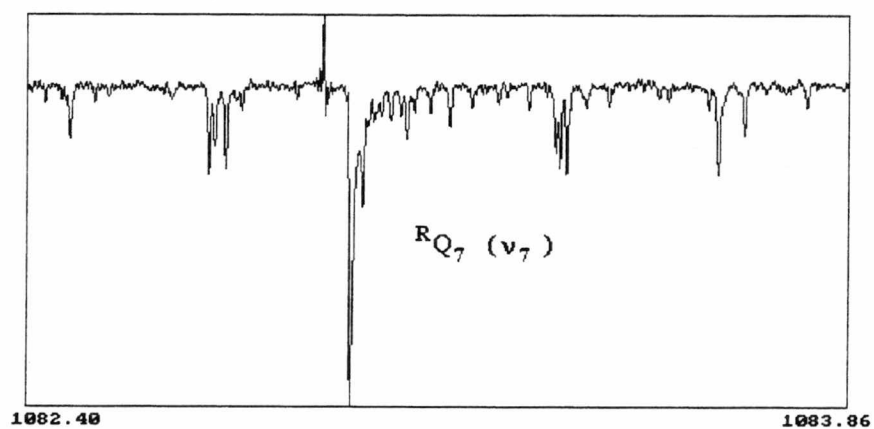


Figure 3.6 (cont.)

Example Q branches from CH_3CN spectrum

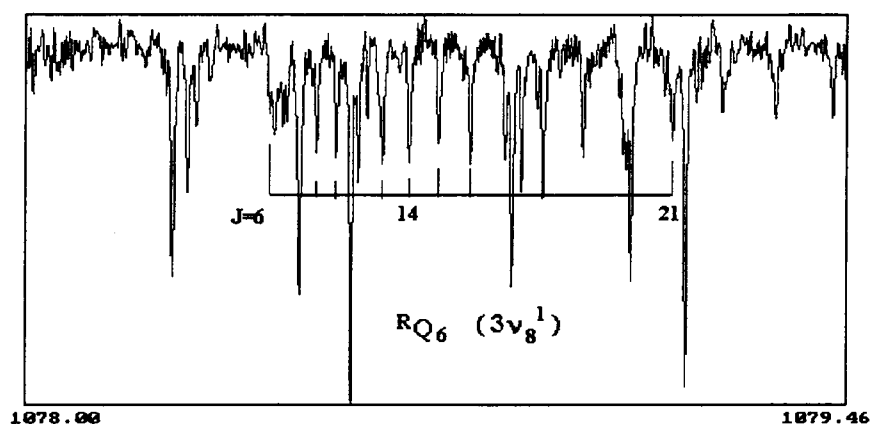


Figure 3.6 (cont.)

Example Q branches from CH_3CN spectrum

wavenumber with increasing J values. So, it is also backward. The ${}^RQ_8$ branch also shows a slight perturbation but it is weak and finally by ${}^RQ_9$ the perturbation is virtually gone.

By fitting the ${}^RQ_6$, ${}^RQ_7$, ${}^RQ_8$ transition energies to a high order polynomial, one can see the perturbation in the value of the constants of the m equation. For instance, the α_B term in the ${}^RQ_7$ fit is oppositely signed compared with other Q branches, hence a backward Q branch. For the ${}^RQ_6$ and ${}^RQ_8$ branches a higher order term dominates at large values of J and causes the Q branch to reverse direction.

TDL Intensity Measurements

Intensity retrieval from absorption spectra is explained by Smith, et al. (Smith, M., C. Rinsland, B. Fridovich, and K. N. Rao, *Intensities and Collision Broadening Parameters from Infrared Spectra, Molecular Spectroscopy: Modern Research, Vol. III*, Academic Press, Inc., 1985). One begins with the Beer-Lambert law which can be written as

$$I(\nu) = I_0 e^{-\alpha(\nu)x} \quad (3.8)$$

where I_0 is the incoming monochromatic radiation and $I(\nu)$ is the reduced radiation after passing through an absorbing gas. The term x is the optical density and is simply the pressure multiplied by the path length and $\alpha(\nu)$ is the absorption coefficient which can be written as

$$\alpha(\nu - \nu_0) = S\phi(\nu - \nu_0) \quad (3.9)$$

where $\varphi(\nu - \nu_0)$ is the line shape function of unit area centered at ν_0 and S is the line strength (intensity) or the integrated absorption coefficient.

Data taken using the TDL system are very near Doppler width so the line shape function can be expressed as

$$\varphi(\nu - \nu_0) = \frac{1}{b_D} \left[\frac{\ln 2}{\pi} \right]^{\frac{1}{2}} e^{-\ln 2 \frac{\nu - \nu_0^2}{b_D^2}} \quad (3.10)$$

where the Doppler width, b_D , is given by

$$b_D = \frac{\nu_0}{c} \left(\frac{2kN_A T \ln 2}{M} \right)^{\frac{1}{2}} \quad \text{or} \quad b_D = 3.581 \times 10^{-7} \nu_0 \left(\frac{T}{M} \right)^{\frac{1}{2}} \quad (3.11)$$

where k is Boltzman's constant, N_A Avogadro's number, T the temperature in Kelvin, c the speed of light, and M the mass of the absorbing gas in atomic mass units (Smith, p.118). It is advantageous to define transmittance $\tau(\nu)$ as

$$\tau(\nu) = \frac{I(\nu)}{I_0} = e^{-\alpha(\nu)x} \quad (3.12)$$

and the area under the line contour curve called the equivalent width or integrated absorption as

$$W = \int_{-\infty}^{\infty} (1 - e^{-\alpha(\nu)x}) d\nu \quad \text{or} \quad W = \int_{-\infty}^{\infty} (1 - \tau(\nu)) d\nu \quad (3.13)$$

and Figure 3.7 graphically depicts the definition of equivalent width.

The equivalent width method can be used to calculate line strengths for Doppler width lines or non-Doppler width lines, but as long as the lines are very near Doppler width, strengths can be calculated by

$$S = \frac{b_D}{x} \left[\frac{\pi}{\ln 2} \right]^{\frac{1}{2}} \ln(\tau(\nu_0)) \quad (3.14)$$

commonly referred to as the direct method or the Jennings method.

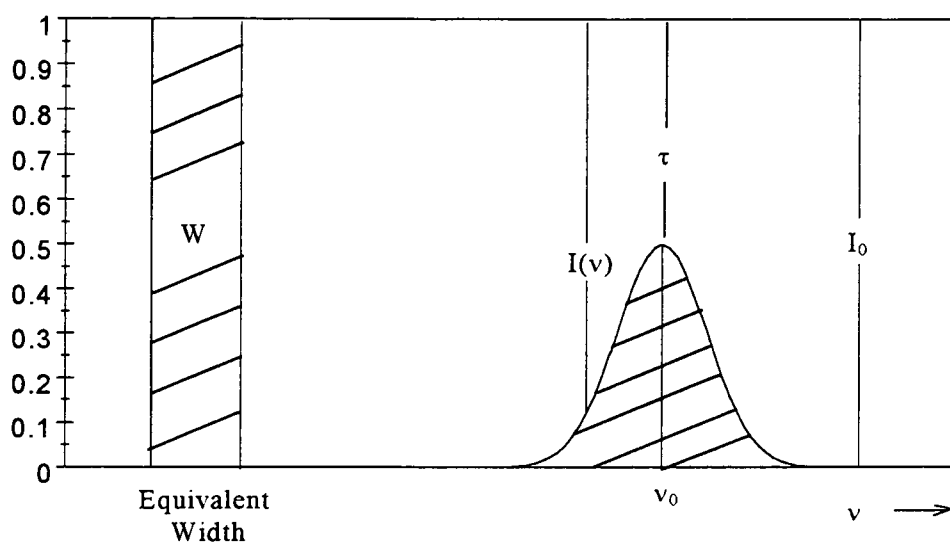


Figure 3.7

Definition of Equivalent Width

Intensity Analysis of TDL Data

Intensity determinations were made using programs written by Dr. Mark Weber, formerly of UTMSL. For the TDL data, N17 was used. This program allows the user to input data from a file created from the download of data from the signal averager. Analysis begins by importing an etalon scan to determine the spacing between data points. This is very crucial since it directly influences the measurement of the half width at half maximum of the absorption line. The user can change the etalon fringe spacing in wavenumbers but the program defaults to 0.01623 wavenumbers. By overlapping a wide data scan with several absorption lines visible with an etalon scan using the same experimental setup, the etalon spacing can be calculated if absorption line positions are known. This can be important since the etalon fringe spacing is temperature sensitive. In this study, the fringe spacing was no greater than 0.0165 wavenumbers and no less than 0.01623 wavenumbers.

The actual absorption data taken using the TDL are analyzed with N17 by first fitting the baseline and the zero transmission level of the spectra. Once these have been established, the program can fit the absorption peak. This program fits the absorption line to an nth order polynomial. The default is a 2nd order polynomial and was used for all fits.

Methyl Cyanide Intensities

To date, there have been no reported values for absorption line intensities for methyl cyanide. The absorption spectra taken using the tunable diode laser (TDL) spectrometer were taken in the 940 cm^{-1} region and the 1000 cm^{-1} region. Several absorption lines were observed for intensity measurements. In addition, data were taken using only one absorption line with several different pressures to determine if

pressure broadening could be detected. The values of pressure in milliTorr and the half width at half maximum (HWHM) in milliwavenumbers for the absorption line $^{\text{P}}\text{P}_5(8)$ at 1010.465 cm^{-1} are shown in Table 3.4 and plotted in Figure 3.8.

Table 3.4
Methyl Cyanide Pressure Broadening Data
for Absorption Data at 1010.465 cm^{-1}

Pressure (mTorr)	HWHM (cm^{-1})
69	0.001337527
101.5	0.0013164
126	0.001425816
150	0.001433466
178.5	0.001497021
202	0.001449475
231.5	0.001435517
252.5	0.001481544
276.5	0.001471185
301.5	0.001499832
331.8	0.001527719
362	0.001566061
380	0.001627802
401.3	0.001628306
429	0.001705374
459.8	0.001716841
487	0.001677392
513.8	0.001742571
551.5	0.001754396
601	0.00177294

Half Width at Half Maximum vs. Pressure
Methyl Cyanide, 1010.46 wavenumbers

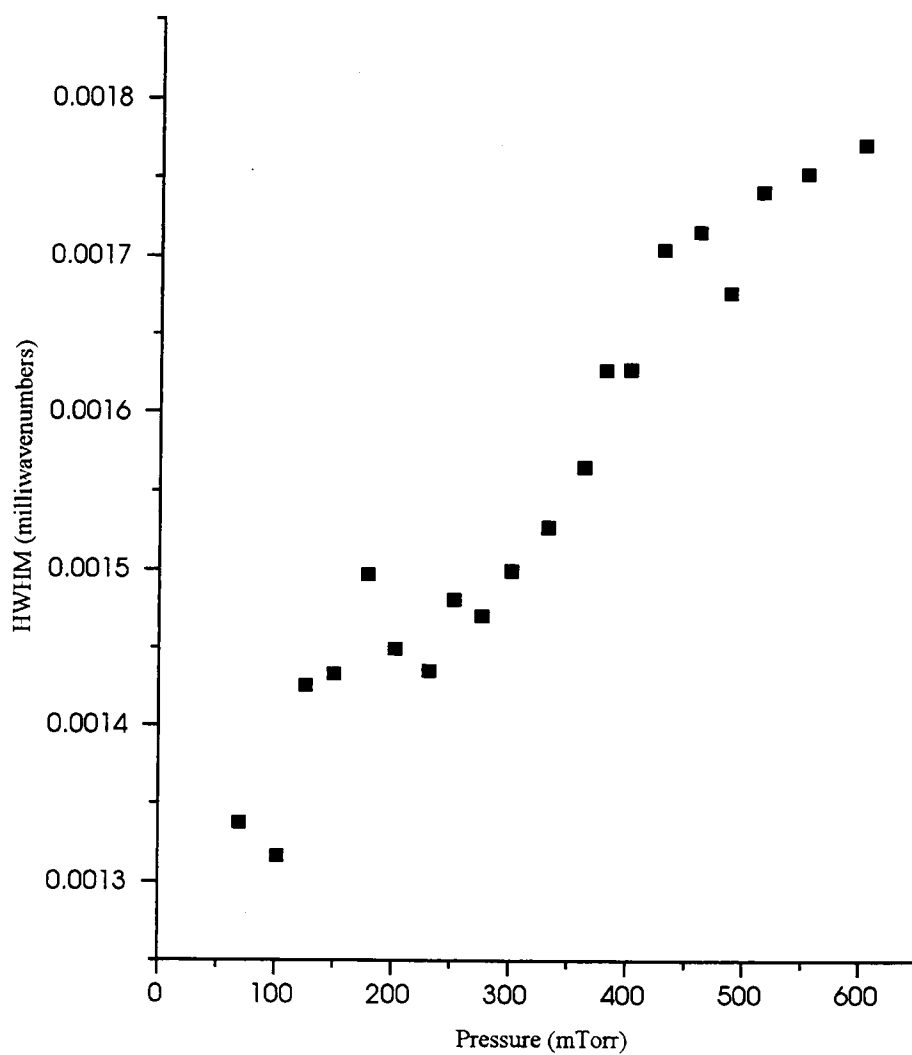


Figure 3.8

Methyl Cyanide Pressure Broadening Curve

The data indicate that there is some pressure broadening. However, due to vibrations in the laser, the data is too erratic to determine a broadening coefficient.

The absorption lines observed for intensity determinations are on the P side of ν_7 and are listed in Table

3.5. Strength values were obtained using the direct method and by using the equivalent width method.

Table 3.5

Methyl Cyanide Intensities from TDL Absorption Spectra

j'	k'	j''	k''	ν_0 (cm^{-1})	S_τ ($\text{cm}^{-2} \text{ atm}^{-1}$)	S_{EW} ($\text{cm}^{-2} \text{ atm}^{-1}$)	%diff S_τ & S_{EW}
0	51	0	52	947.8774	0.0002787()	0.0002829()	-1.492087
6	52	6	53	948.076	0.0003282()	0.0003303()	-0.648064
6	53	6	54	948.5201	0.0002388()	0.0001896()	-22.96365
6	54	6	55	948.9569	0.0002857()	0.0002447()	15.484364
3	54	3	55	949.1449	0.0005934(862)	0.0005206(209)	7.7039802
2	34	1	33	1010.332	0.001634(181)	0.001701(198)	7.7039802
5	8	4	7	1010.465	0.002861(127)	0.003036(113)	7.7039802
3	25	2	24	1010.549	0.004148(770)	0.004202(920)	7.7039802

Although there is good agreement between strength values calculated by the equivalent width method and by the direct method for many of the lines, most lines have values for the half width at half maximum which are significantly far from Doppler. As mentioned before, the instability of the laser was causing the lines to be artificially broadened. This problem was eventually corrected. The laser was moved to a separate table as discussed in Chapter 2. This did not have the desired result although vibration sensitivity was reduced. Data taken still exhibited half widths significantly greater than the Doppler width. Testing of the laser current controller showed a noisy current ramp being sent to the diode laser.

The noisy ramp essentially caused the diode laser to scan frequency in random fashion instead of linearly. The signal averager averaged the scanned points and this caused the absorption lines to be artificially broadened. Single scans often gave good half widths but with a poor signal to noise ratio.. The noisy ramp was caused by a ground loop and by grounding everything to the same point the ramp noise was reduced to approximately zero. Subsequent data proved to be vastly improved. It was not possible to include the new CH₃CN data in this work.

Ethylene Intensities

Absorption lines of ethylene (C₂H₄) were measured using the TDL spectrometer. A 48.26 cm cell was used to obtain the absorption spectra. The problem that plagued the methyl cyanide experiment was solved in time to obtain ethylene spectra for making strength determinations. Several lines from the ν_7 band of ethylene were measured and the results are given in Table 3.6. In addition to the TDL intensities, absorption lines from the KPNO FTS data were measured using programs written by Dr. Mark Weber of Goddard Space Flight Center. The programs are BLOCKPD, which takes a Kitt Peak data file and breaks it into smaller files that can be read into the analysis programs, FTDPY, which reads in a file created by BLOCKPD and allows the user to set the baseline for the spectra, perform a sinc interpolation of the data if it is overresolved, and prepare for a least squares fitting, and FTFIT, which performs a least squares fit of the absorption line(s) and returns a value for the intensity of each line. FTFIT allows the user to fit values of strength and line center frequency as well as broadening coefficients. In this study, the line center frequency and strength were fit. A detailed discussion of the analysis programs can be found in the accompanying documentation of the programs. Selected line strengths for the 940 cm⁻¹ to 960 cm⁻¹ region are listed in Appendix E, Table E.1 with transition assignments. The FTS strengths have been rescaled using the calibration shown in Figure 3.9. Strengths calculated with the equivalent width method from

TDL measurements were plotted against FTS strength measurements and a calibration equation was determined.

Table 3.6

Strengths from TDL and recalibrated FTS data for ethylene absorption lines. Errors in strengths are standard deviations and are given parenthetically in the last digits of the strengths.

$\langle S \rangle$ are averages of the S_{EW} and S_t . Strengths are scaled to 296 K.

J'	Ka'	Kc'	J''	Ka''	Kc''	Frequency (cm ⁻¹)	S_{EW} cm ⁻² atm ⁻¹	S_t cm ⁻² atm ⁻¹	$\langle S \rangle$ cm ⁻² atm ⁻¹	S(FTS) cm ⁻² atm
11	1	10	11	2	10	941.84782	0.8238(283)	0.8222(20)	0.8230(150)	0.8240(190)
8	2	6	9	1	8	942.10127	0.1292(65)	0.1302(88)	0.1297(76)	0.1157(45)
3	1	2	4	0	4	946.11957	0.2410()	0.2314()	0.2362()	0.2400(81)
6	1	6	5	2	4	946.17457	0.1094(23)	0.1122(7)	0.1108(15)	0.1210(71)
6	0	6	6	1	6	946.28257	0.5707(41)	0.5601(86)	0.5654(63)	0.5699(110)
13	3	10	12	4	8	946.76234	0.1504()	0.1337()	0.1421()	0.1461(64)
6	1	6	6	0	6	951.37167	1.3851(277)	*	1.3851(277)	1.4155(237)
5	1	5	5	0	5	951.73936	0.5267(302)	0.5232(143)	0.5250(223)	0.4778(142)
7	3	4	7	2	6	970.02301	0.4813(288)	0.4672(132)	0.4743(210)	0.4715(273)

Ethylene Strength Calibration Curve

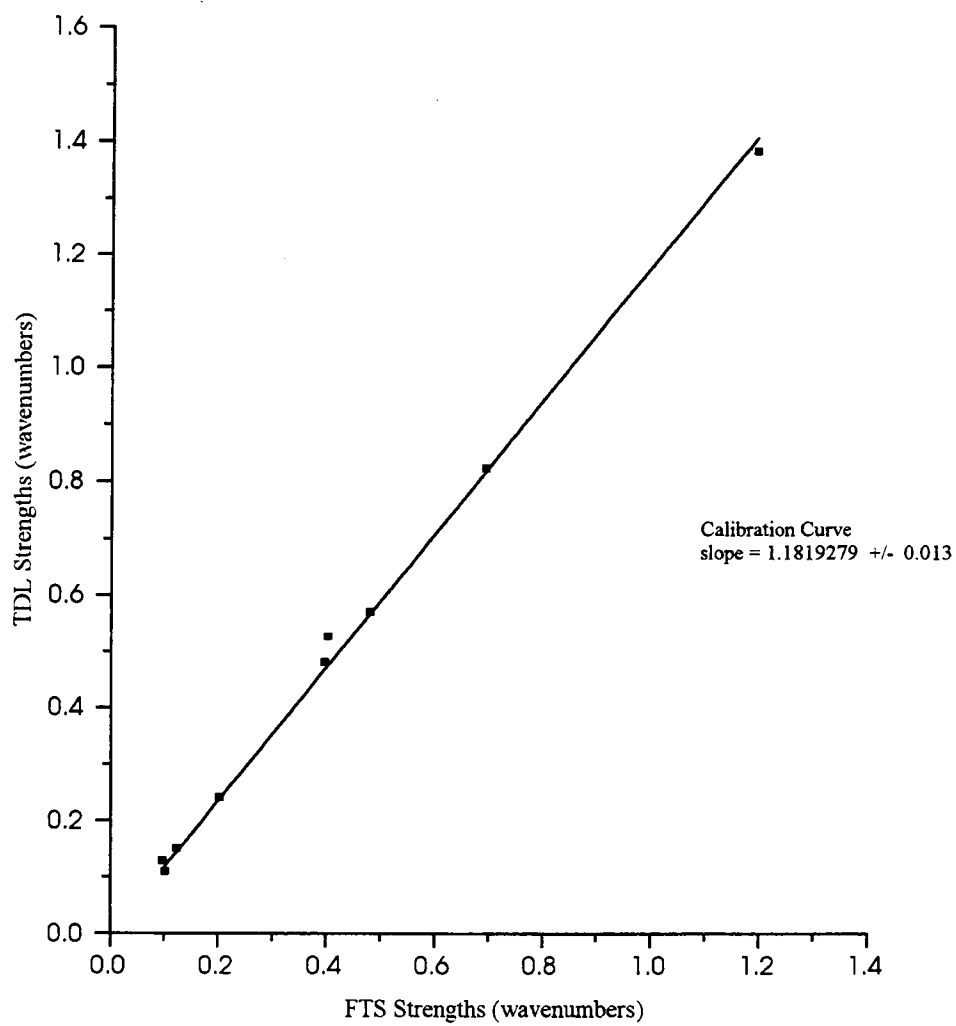


Figure 3.9

Ethylene FTS Strength Calibration Curve

Chapter 4

Future Work and Comparison of Results

Future Work on Methyl Cyanide and Ethylene

The data reported in this work on methyl cyanide are just the beginning of the work necessary to aid astronomers. The transition energy assignments of the ν_7 band are, for the most part, completed. However, absorption line intensities are needed to further model the molecule and its spectrum. As of this writing, no intensities have been reported and the data reported in this work need to be retaken with the new TDL experimental design. In addition to basic intensity measurements, a value for the broadening coefficient needs to be determined. The data in this thesis indicate that the broadening coefficient is very large compared to that for methane. Hydrogen and nitrogen broadening experiments should also be performed to assist the planetary atmospheric modellers in their simulation of the Titan atmosphere. The TDL is currently able to determine line strengths from the $2\nu_8^0$, ν_4 and ν_7 bands, so a wide range of intensity measurements can quickly be made. The current experimental setup also makes it possible to use different path lengths which insures the validity of the data. Additional work on ethylene must be done in the areas of pressure, nitrogen, and hydrogen broadening.

By determining more information on these molecules, it will be possible to better model planetary atmospheres of Jupiter and Saturn and of Titan. The data on methyl cyanide can help to identify and determine population and temperature of molecular clouds.

Comparison to Recent Results

Unfortunately, no work has been done on intensity measurements of methyl cyanide. Attempts to measure intensities of the FTS data proved to be futile. The spectra were very noisy and there appeared to be some broadening of the absorption lines.

Ethylene data have been reported by Ewing (Ewing, Alan, Masters thesis, University of Tennessee, 1993) and Reuter (Reuter, D. and J. M. Sirota, *Absolute Intensities and Foreign Gas Broadening Coefficients of the $11_{1,10} \leftarrow 11_{2,10}$ and $18_{0,18} \leftarrow 18_{1,18}$ Lines in the ν_7 Band of C_2H_4* , **Journal of Quantitative Spectroscopic Radiative Transfer**, Vol. 50, No. 5, p. 477-482, 1993). Comparison with this work is made in Table 4.1. Strengths are given in units of $\text{cm}^{-2} \text{atm}^{-1}$ and the frequencies are in wavenumbers. Agreement is not as good as hoped but there needs to be more measurements of the line strengths of ethylene.

Table 4.1

Comparison of absorption line strengths. Errors, where available, are given in parenthesis.

Strengths are given in units of $\text{cm}^{-2} \text{atm}^{-1}$ and ν_0 is in wavenumbers.

J'	K _a '	K _c '	J''	K _a ''	K _c ''	ν_0 (cm^{-1})	S (this work) ($\text{cm}^{-2} \text{atm}^{-1}$)	S (Ewing) ($\text{cm}^{-2} \text{atm}^{-1}$)	S (Reuter) ($\text{cm}^{-2} \text{atm}^{-1}$)
11	1	10	11	2	10	941.8478	0.8283(283)	0.968(636)	0.960(15)
5	1	5	5	0	5	951.7394	0.5267(302)	0.4889(306)	0.484(20)
18	1	18	18	0	18	949.1074	0.6314(129) *	0.697() *	0.699(10)
12	1	12	12	0	12	948.2277	0.8983(246) *	0.965() *	0.99 ()

* denotes rescaled FTS strength

Conclusion

The goal of this study was to measure line strengths of the ν_7 band of ethylene and the ν_7 and ν_4 bands of methyl cyanide. Strengths were measured from data taken at the UTMSL TDL spectrometer and KPNO FTS. Line strengths for methyl cyanide were inconclusive due to problems with the TDL spectrometer. Although this problem was rectified, there was no time to report the results for methyl cyanide. In addition, transition energies for the ν_7 band of methyl cyanide were determined. The line strengths from the TDL and the rescaled FTS values seem to be in good agreement and are also in good agreement with independent measurements. This seems to indicate that the method is sound and will be able to produce additional measurements with good agreement as well.

LIST OF REFERENCES

LIST OF REFERENCES

- Abeles, F. B. and H. E. Heggstad, *Ethylene: An Urban Air Pollutant*, **Journal of Air Pollution Control Association**, **23**, 517, 1973.
- Abrams, Mark, Ph.D. dissertation, University of California, Berkley, 1990.
- Allen, H. and P. Cross, **Molecular Vib-Rotors**, p. 151, Wiley and Sons, Inc., New York, 1963.
- Arnold, F., H. Böhringer, and G. Henschen, *Composition Measurements of Stratospheric Positive Ions*, **Geophysical Research Letters**, Vol. 5, No.8, p. 653—656, 1978.
- Becker, K. H. and A. Ionescu, *Acetonitrile In The Lower Atmosphere*, **Geophysical Research Letters**, Vol. 9, No. 12, p. 1349—1351, 1982.
- Betz, A. L., *Ethylene in IRC +10216*, **The Astrophysical Journal**, **244**, L103-L105, 1981.
- Blass, W. E., S. Daunt, A. Ewing, S. Hager, J. Hillman, D. Jennings, L. Jennings, D. Reuter, L. Senesac, and M. Weber, **An Ethylene Atlas**, to be published, 1995.
- Blass, W. E. and J. Hillman, private communication.
- Blass, W. E., Ph.D. dissertation, Michigan State University, 1963.
- Brown, F., D. Dangoisse, and J. Demaison, *The Rotational Spectrum of CH₃CN above 1000 GHz*, **Journal of Molecular Spectroscopy**, **129**, 483-485, 1988.
- Carlotti, Di Lonardo, Fusina, and Carli, *The Far-Infrared Spectrum of Methyl Cyanide, CH₃CN*, **Journal of Molecular Spectroscopy**, **129**, 314-325, 1988.
- Clark, F. O., R. D. Brown, P. D. Godfrey, J. W. V. Storey, and D. R. Johnson, *Detection of Interstellar Vibrationally Excited Cyanoacetylene*, **The Astrophysical Journal**, **210**, L139-L140, 1976.
- Cohen-Tannoudji, C., B. Diu, and F. Laloe, **Quantum Mechanics**, Vol. I, p. 512, Wiley & Sons, New York, 1977.
- Dakhil, M., Ph.D. dissertation, University of Tennessee, 1983.
- Daunt, Stephen, Ph.D. dissertation, Queen's University, Canada, 1976.
- Duncan, J. L., *The calculation of force constants and normal coordinates —V*, **Spectrochimica Acta**, Vol. 20, p. 1197, 1964.
- Ewing, Alan, Masters thesis, University of Tennessee, 1993.
- Gillett, F. C., *Further Observations of the 8-13 Micron Spectrum of Titan*, **The Astrophysical Journal**, **201**, L41-L43, 1975.

Gordy, Walter and Robert L. Cook, Microwave Molecular Spectroscopy, Interscience Publishers, New York, 1970.

Herzberg, G., Infrared and Raman Spectra of Polyatomic Molecules, p.26, Van Nostrand Reinhold Company, NY, 1945.

Jennings, D. E., W. E. Blass, and N. M. Gailar, *Absorption cell: a modified multiple-traversal device*, **Applied Optics**, Vol. 15, No. 4, p. 864, 1976.

Kostuik, T., F. Espenak, M. Mumma, and P. Romani, *Infrared Studies of Hydrocarbons on Jupiter*, **Infrared Physics**, 29, 198-204, 1989.

Kroto, H. W., Molecular Rotation Spectra, John Wiley & Sons, New York, 1975.

Loren, R. B., L. Mundy, and N. R. Erickson, *High Temperature Methyl Cyanide in Orion Molecular Cloud I*, **The Astrophysical Journal**, 250, 573-578, 1981.

Maguire, W. C., R. A. Hanel, D. E. Jennings, V. G. Kunde and R. E. Samuelson, **Nature**, 292, 683-686, 1981.

Mori, Y., T. Nakagawa, and K. Kuchitsu, *Vibration-Rotation Spectra of CH_3CN : The ν_7 Band and Its Hot Bands near 1040 cm^{-1}* , **Journal of Molecular Spectroscopy**, 104, 388-401, 1984.

Muller, C., *Acetonitrile in the Earth's Atmosphere: An Upper Limit Deduced from Infrared Solar Spectra*, **Bull. Cl. Sc. Acad. Roy. Belg.**, p. 225—229, 1985.

Parker, F. W., A. H. Nielsen, and W. H. Fletcher, *The Infrared Absorption Spectrum of Methyl Cyanide Vapor*, **Journal of Molecular Spectroscopy**, 1, 107-123, 1957.

Rackley, S. A., R. J. Butcher, M. Römheld, S. M. Freund, and T. Oka, *Laser Stark Spectroscopy of Methyl Cyanide in the $10\text{-}\mu\text{m}$ Region: Analysis of the ν_4 and ν_7 Bands, and the ν_7 , $3\nu_8^1$ Interaction*, **Journal of Molecular Spectroscopy**, 92, p. 203—217, 1982.

Reuter, D. and J. M. Sirota, *Absolute Intensities and Foreign Gas Broadening Coefficients of the $11_{1,10} \leftarrow 11_{2,10}$ and $18_{0,18} \leftarrow 18_{1,18}$ Lines in the ν_7 Band of C_2H_4* , **Journal of Quantitative Spectroscopic Radiative Transfer**, Vol. 50, No. 5, p. 477-482, 1993.

Smith, M., C. Rinsland, B. Fridovich, and K. N. Rao, *Intensities and Collision Broadening Parameters from Infrared Spectra*, **Molecular Spectroscopy: Modern Research, Vol. III**, Academic Press, Inc., 1985.

Snider, J. R. and G. A. Dawson, *Surface Acetonitrile Near Tucson, Arizona*, **Geophysical Research Letters**, Vol. 11, No. 3, p.241—242, 1984.

Solomon, P. M., K. B. Jefferts, A. A. Penzias, and R. W. Wilson, *Detection of Millimeter Emission Lines from Interstellar Methyl Cyanide*, **The Astrophysical Journal**, 168, L107-110, 1971.

Solomon, P. M., A. A. Penzias, K. B. Jefferts, and R. W. Wilson, *Millimeter Emission Lines of Polyatomic Molecules in Sagittarius B2*, **The Astrophysical Journal**, 185, L63-L66, 1973.

Strobel, D. F., *The Photochemistry of Hydrocarbons in the Atmosphere of Titan*, **Icarus**, **21**, 466, 1974.

Swindle, D. J., and J. A. Roberts, *Linewidth Parameters in the Rotational Spectrum of Methyl Cyanide*, **Journal of Molecular Spectroscopy**, **77**, No. 1, July 1979.

Tolonen, A.-M., M. Koivusaari, R. Paso, J. Schroderus, S. Alanko, and R. Anttila, *The Infrared Spectrum of Methyl Cyanide between 850 and 1150 cm^{-1} : Analysis of the ν_4 , ν_7 , and $3\nu_8^{-1}$ bands with Resonances*, **Journal of Molecular Spectroscopy**, **160**, 554-565, 1993.

Weber, Mark, Ph.D. dissertation, University of Tennessee, 1992.

APPENDICES

Appendix A

Assignments for the R side of the ν_7 band and the $3\nu_8^1$, $K = 6$, band of methyl cyanide from data obtained from Kitt Peak National Observatory's Fourier transform spectrometer are listed in Table A.1. All energies are reported in wavenumbers. $^R P_K(J)$ absorption lines were assigned with the aid of Alan Ewing of UTMSL.

Table A.1

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	1	6	0	7	17.826928250	1041.1037	1041.108643
7	1	11	2	10	45.440209780	1041.1204	1041.125343
7	2	15	1	16	93.388120530	1041.1149	1041.119843
7	2	20	3	19	148.600392700	1041.16035	1041.165293
7	3	24	2	25	228.481207400	1041.1992	1041.204144
7	3	29	4	28	311.263947700	1041.22557	1041.230514
7	4	33	3	34	423.029299300	1041.30016	1041.305104
7	4	40	5	39	581.743597700	1041.30016	1041.305104
7	5	47	6	46	814.704226400	1041.39368	1041.398625
7	1	7	0	8	22.122462700	1041.70936	1041.714306
7	1	10	2	9	38.690486480	1041.73280	1041.737746
7	2	16	1	17	103.204236500	1041.74024	1041.745186
7	2	19	3	18	136.331709500	1041.78137	1041.786316
7	3	25	2	26	243.812738500	1041.80331	1041.808256
7	3	28	4	27	293.482546900	1041.84915	1041.854097
7	4	34	3	35	443.868252300	1041.90077	1041.905717
7	4	39	5	38	557.236170200	1041.93575	1041.940697
7	5	46	6	45	785.927361300	1042.02223	1042.027178
7	1	8	0	9	27.031583980	1042.3195	1042.324449
7	1	9	2	8	32.554267720	1042.34867	1042.353619
7	2	17	1	18	113.633575000	1042.34867	1042.353619
7	2	18	3	17	124.676084300	1042.40110	1042.406049
7	3	26	2	27	259.756858700	1042.40708	1042.412029

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ (K=6) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground.State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	3	27	4	26	276.313488800	1042.47212	1042.47707
7	4	35	3	36	465.318893500	1042.50078	1042.50573
7	1	9	0	10	32.554267720	1042.92965	1042.934602
7	2	18	1	19	124.676084300	1042.95392	1042.958872
7	1	8	2	7	27.031583980	1042.9714	1042.976352
7	3	27	2	28	276.313488800	1043.01055	1043.015502
7	2	17	3	16	113.633575000	1043.02069	1043.025642
7	3	26	4	25	259.756858700	1043.09489	1043.099843
7	4	37	5	36	510.054812700	1043.18231	1043.187263
7	1	10	0	11	38.690486480	1043.53976	1043.544715
7	2	19	1	20	136.331709500	1043.56038	1043.565335
7	1	7	2	6	22.122462700	1043.58279	1043.587745
7	3	28	2	29	293.482546900	1043.61343	1043.618385
7	2	16	3	15	103.204236500	1043.64048	1043.645435
7	4	37	3	38	510.054812700	1043.7001	1043.705055
7	3	25	4	24	243.812738500	1043.71758	1043.722536
7	4	36	5	35	487.381116800	1043.80794	1043.812896
7	1	11	0	12	45.440209780	1044.14869	1044.153648
7	2	20	1	21	148.600392700	1044.16638	1044.171338
7	1	6	2	5	17.826928250	1044.19852	1044.203478
7	3	29	2	30	311.263947700	1044.2157	1044.220658
7	2	15	3	14	93.388120530	1044.25966	1044.264618
7	4	38	3	39	533.339869000	1044.29918	1044.304138
7	3	24	4	23	228.481207400	1044.34002	1044.344979
7	4	35	5	34	465.318893500	1044.43280	1044.437759
7	5	42	6	41	676.922413400	1044.53077	1044.535729
7	1	12	0	13	52.803404110	1044.75751	1044.762471
7	0	3	1	4	3.682088711	1044.7781	1044.783061
7	2	21	1	22	161.482073200	1044.77116	1044.776121
7	1	5	2	4	14.145001950	1044.8191	1044.824061
7	3	30	2	31	329.657602900	1044.81744	1044.822401

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground.State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	2	14	3	13	84.185275820	1044.87827	1044.883231
7	3	23	4	22	213.762341500	1044.96185	1044.966811
7	4	34	5	33	443.868252300	1045.05796	1045.062922
7	5	41	6	40	651.197478900	1045.15550	1045.160462
7	6	50	7	49	958.808568300	1045.30350	1045.308463
7	1	13	0	14	60.780032900	1045.36594	1045.370903
7	0	4	1	5	6.136794197	1045.38163	1045.386593
7	2	22	1	23	174.976686900	1045.38163	1045.386593
7	3	31	2	32	348.663421400	1045.41914	1045.424104
7	1	4	2	3	11.076702110	1045.4343	1045.439264
7	2	13	3	12	75.595748030	1045.49653	1045.501494
7	3	22	4	21	199.656213800	1045.58332	1045.588284
7	4	33	5	32	423.029299300	1045.68220	1045.687165
7	5	40	6	39	626.083324600	1045.78180	1045.786765
7	6	49	7	48	928.208544700	1045.91840	1045.923366
7	1	14	0	15	69.370056520	1045.97357	1045.978536
7	2	23	1	24	189.084166700	1045.98072	1045.985686
7	0	5	1	6	9.205153193	1045.99227	1045.997236
7	3	32	2	33	368.281308900	1046.02065	1046.025617
7	1	3	2	2	8.622043949	1046.0491	1046.054067
7	4	41	3	42	606.862030300	1046.09326	1046.098227
7	2	12	3	11	67.619579800	1046.11530	1046.120267
7	3	21	4	20	186.162894100	1046.20478	1046.209747
7	4	32	5	31	402.802137900	1046.30543	1046.310398
7	5	39	6	38	601.580074700	1046.40710	1046.412068
7	6	48	7	47	898.218078300	1046.53480	1046.539769
7	1	15	0	16	78.573432310	1046.58319	1046.588159
7	0	6	1	7	12.887150460	1046.6125	1046.629969
7	3	33	2	34	388.511167900	1046.62134	1046.626309
7	2	11	3	10	60.256810720	1046.738	1046.74297
7	3	20	4	19	173.282449400	1046.82559	1046.83056

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground.State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	4	31	5	30	383.186868300	1046.92992	1046.934891
7	5	38	6	37	577.687850400	1047.03150	1047.036471
7	6	47	7	46	868.837317300	1047.15360	1047.158572
7	1	16	0	17	88.390114560	1047.18878	1047.193752
7	2	25	1	26	219.137441900	1047.18878	1047.193752
7	0	7	1	8	17.182767700	1047.21158	1047.216552
7	3	34	2	35	409.352898200	1047.22195	1047.226922
7	1	55	2	55	948.791149100	1047.29011	1047.295083
7	1	54	2	54	915.123679800	1047.31217	1047.317143
7	1	53	2	53	882.065355100	1047.33373	1047.338703
7	1	52	2	52	849.616339600	1047.35229	1047.357263
7	2	10	3	9	53.507477330	1047.35229	1047.357263
7	1	50	2	50	786.546879900	1047.39358	1047.398553
7	1	49	2	49	755.926750000	1047.41346	1047.418433
7	1	48	2	48	725.916557600	1047.43222	1047.437193
7	3	19	4	18	161.014943600	1047.44556	1047.450533
7	1	46	2	46	667.726580300	1047.46899	1047.473963
7	1	45	2	45	639.547085000	1047.48689	1047.491863
7	1	44	2	44	611.978106800	1047.50417	1047.509144
7	1	43	2	43	585.019782900	1047.52159	1047.526564
7	1	42	2	42	558.672247300	1047.53799	1047.542964
7	1	41	2	41	532.935631300	1047.55415	1047.559124
7	4	30	5	29	364.183587600	1047.55415	1047.559124
7	1	40	2	40	507.810062800	1047.57006	1047.575034
7	1	39	2	39	483.295667000	1047.58562	1047.590594
7	1	38	2	38	459.392565800	1047.60097	1047.605944
7	1	37	2	37	436.100878000	1047.61536	1047.620334
7	1	36	2	36	413.420719500	1047.62996	1047.634934
7	1	35	2	35	391.352203200	1047.64369	1047.648664
7	1	34	2	34	369.895438800	1047.65716	1047.662134
7	5	37	6	36	554.406769900	1047.65716	1047.662134

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground.State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	1	33	2	33	349.050533000	1047.67022	1047.675194
7	1	32	2	32	328.817589400	1047.68305	1047.688024
7	1	31	2	31	309.196708700	1047.69531	1047.700284
7	1	30	2	30	290.187988400	1047.70741	1047.712385
7	1	29	2	29	271.791523000	1047.71898	1047.723955
7	1	28	2	28	254.007403900	1047.73011	1047.735085
7	1	27	2	27	236.835719500	1047.74083	1047.745805
7	1	26	2	26	220.276555300	1047.75148	1047.756455
7	1	25	2	25	204.329993400	1047.76132	1047.766295
7	1	24	2	24	188.996113200	1047.77091	1047.775885
7	6	46	7	45	840.066407000	1047.77091	1047.775885
7	1	23	2	23	174.274990900	1047.78026	1047.785235
7	1	22	2	22	160.166699500	1047.78995	1047.794925
7	1	17	0	18	98.820054490	1047.79695	1047.801925
7	1	21	2	21	146.671309200	1047.80575	1047.810725
7	1	20	2	20	133.788887100	1047.81343	1047.818405
7	0	8	1	9	22.091983580	1047.82074	1047.825715
7	3	35	2	36	430.806396100	1047.82074	1047.825715
7	1	18	2	18	109.863200300	1047.82729	1047.832265
7	1	17	2	17	98.820054490	1047.83362	1047.838595
7	2	9	3	8	47.371613130	1047.96704	1047.972016
7	3	18	4	17	149.360437500	1048.06604	1048.071016
7	4	29	5	28	345.792390000	1048.17546	1048.180437
7	5	36	6	35	531.736948400	1048.28059	1048.285567
7	2	27	1	28	251.641301800	1048.39568	1048.400658
7	1	18	0	19	109.863200300	1048.4017	1048.406678
7	3	36	2	37	452.871555400	1048.42068	1048.425658
7	0	9	1	10	27.614773720	1048.4431	1048.448078
7	2	8	3	7	41.849248560	1048.5891	1048.594079
7	3	17	4	16	138.318988900	1048.6914	1048.696379
7	4	28	5	27	328.013366600	1048.79774	1048.80272

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	5	35	6	34	509.678498000	1048.90449	1048.90947
7	2	28	1	29	268.812001100	1048.99812	1049.003101
7	1	19	0	20	121.519497200	1049.00694	1049.011921
7	6	44	7	43	784.354703400	1049.00694	1049.011921
7	3	37	2	38	475.548266400	1049.01965	1049.024631
7	0	10	1	11	33.751110680	1049.03625	1049.041231
7	1	1	2	2	5.553698394	1049.11276	1049.117741
7	2	7	3	6	36.940411040	1049.2054	1049.210382
7	3	16	4	15	127.890652600	1049.30567	1049.310652
7	4	27	5	26	310.846605400	1049.42030	1049.425283
7	5	34	6	33	488.231527700	1049.52810	1049.533083
7	2	29	1	30	286.595100700	1049.59989	1049.604874
7	6	43	7	42	757.414185200	1049.61223	1049.617214
7	1	20	0	21	133.788887100	1049.61827	1049.623254
7	3	38	2	39	498.836416500	1049.61827	1049.623254
7	0	11	1	12	40.500963980	1049.6436	1049.648584
7	1	2	2	3	6.781039663	1049.71489	1049.719874
7	2	6	3	5	32.645124920	1049.81570	1049.820685
7	3	15	4	14	118.075480100	1049.92491	1049.929895
7	4	26	5	25	294.292191500	1050.04250	1050.047486
7	5	33	6	32	467.396143700	1050.15102	1050.156006
7	2	30	1	31	304.990512100	1050.20166	1050.206646
7	1	21	0	22	146.671309200	1050.21722	1050.222206
7	3	39	2	40	522.735890200	1050.21722	1050.222206
7	6	42	7	41	731.084067900	1050.23390	1050.238887
7	0	12	1	13	47.864300080	1050.2705	1050.275487
7	1	3	2	4	8.622043949	1050.3421	1050.347087
7	2	5	3	4	28.963411520	1050.42980	1050.434787
7	3	14	4	13	108.873520300	1050.54316	1050.548148
7	4	25	5	24	278.350206800	1050.66309	1050.668079
7	5	32	6	31	447.172448800	1050.77575	1050.780739

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	2	31	1	32	323.998144100	1050.80275	1050.807739
7	1	22	0	23	160.166699500	1050.81393	1050.818919
7	3	40	2	41	547.246568800	1050.81393	1050.818919
7	6	41	7	40	705.364481300	1050.83780	1050.842789
7	0	13	1	14	55.841082400	1050.85631	1050.861299
7	1	4	2	5	11.076702110	1050.94895	1050.95394
7	3	13	4	12	100.284818700	1051.16204	1051.167031
7	5	26	4	26	338.681140400	1051.27481	1051.279801
7	4	24	5	23	263.020730200	1051.28509	1051.290082
7	5	31	6	30	427.560543200	1051.39466	1051.399652
7	2	32	1	33	343.617902200	1051.40303	1051.408022
7	3	41	2	42	572.368330500	1051.4111	1051.416092
7	1	23	0	24	174.274990900	1051.42717	1051.432162
7	0	14	1	15	64.431271320	1051.46144	1051.466432
7	6	40	7	39	680.255552400	1051.50950	1051.514493
7	1	5	2	6	14.145001950	1051.56011	1051.565103
7	3	12	4	11	92.309417860	1051.77991	1051.784904
7	4	23	5	22	248.303837700	1051.90622	1051.911214
7	2	33	1	34	363.849688800	1052.00563	1052.010625
7	3	42	2	43	598.101050700	1052.00563	1052.010625
7	5	30	6	29	408.560523800	1052.0170	1052.021995
7	1	24	0	25	188.996113200	1052.03129	1052.036285
7	0	15	1	16	73.634824160	1052.0952	1052.100195
7	1	6	2	7	17.826928250	1052.176	1052.180996
7	6	39	7	38	655.757405100	1052.09960	1052.104595
7	3	11	4	10	84.947357350	1052.4027	1052.407697
7	4	22	5	21	234.199602100	1052.52441	1052.529407
7	3	43	2	44	624.444601400	1052.57327	1052.578268
7	2	34	1	35	384.693403600	1052.60319	1052.608188
7	1	25	0	26	204.329993400	1052.63534	1052.640338
7	5	29	6	28	390.172484400	1052.63534	1052.640338

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	0	16	1	17	83.451695190	1052.67073	1052.675728
7	1	7	2	8	22.122462700	1052.78164	1052.786639
7	2	53	3	53	896.834319800	1052.92927	1052.934269
7	2	52	3	52	864.387126800	1052.95263	1052.957629
7	2	51	3	51	832.549372300	1052.97332	1052.97832
7	2	50	3	50	801.321215000	1052.9944	1052.9994
7	2	49	3	49	770.702810200	1053.01479	1053.01979
7	3	10	4	9	78.198673650	1053.01479	1053.01979
7	2	48	3	48	740.694310400	1053.03409	1053.03909
7	2	47	3	47	711.295864900	1053.05352	1053.05852
7	2	46	3	46	682.507619900	1053.07284	1053.07784
7	2	45	3	45	654.329718700	1053.0912	1053.0962
7	2	44	3	44	626.762301500	1053.10976	1053.11476
7	2	43	3	43	599.805505300	1053.12719	1053.13219
7	2	42	3	42	573.459464300	1053.14492	1053.14992
7	4	21	5	20	220.708093300	1053.14492	1053.14992
7	2	41	3	41	547.724309500	1053.16149	1053.16649
7	2	40	3	40	522.600168800	1053.17783	1053.18283
7	2	39	3	39	498.087167200	1053.19379	1053.198791
7	3	44	2	45	651.398851900	1053.19379	1053.198791
7	2	35	1	36	406.148942900	1053.20102	1053.206021
7	2	38	3	38	474.185426500	1053.20968	1053.214681
7	2	37	3	37	450.895065600	1053.22471	1053.229711
7	1	26	0	27	220.276555300	1053.23885	1053.243851
7	2	36	3	36	428.216200100	1053.23885	1053.243851
7	2	35	3	35	406.148942900	1053.25434	1053.259341
7	5	28	6	27	372.396516000	1053.25434	1053.259341
7	2	34	3	34	384.693403600	1053.26825	1053.273251
7	0	17	1	18	93.881835630	1053.2744	1053.279401
7	2	33	3	33	363.849688800	1053.28172	1053.286721
7	2	32	3	32	343.617902200	1053.29471	1053.299711

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	2	31	3	31	323.998144100	1053.30748	1053.312481
7	2	30	3	30	304.990512100	1053.31966	1053.324661
7	6	37	7	36	608.593936000	1053.31966	1053.324661
7	2	29	3	29	286.595100700	1053.33209	1053.337091
7	2	28	3	28	268.812001100	1053.34335	1053.348351
7	2	27	3	27	251.641301800	1053.35474	1053.359741
7	2	26	3	26	235.083088000	1053.36554	1053.370541
7	2	25	3	25	219.137441900	1053.37582	1053.380821
7	2	24	3	24	203.804442800	1053.38568	1053.390681
7	1	8	2	9	27.031583980	1053.39376	1053.398762
7	2	22	3	22	174.976686900	1053.40425	1053.409252
7	2	21	3	21	161.482073200	1053.41291	1053.417912
7	2	20	3	20	148.600392700	1053.4213	1053.426302
7	2	19	3	19	136.331709500	1053.42904	1053.434042
7	2	18	3	18	124.676084300	1053.43644	1053.441442
7	2	17	3	17	113.633575000	1053.44366	1053.448662
7	2	16	3	16	103.204236500	1053.45024	1053.455242
7	2	15	3	15	93.388120530	1053.45685	1053.461852
7	3	9	4	8	72.063400220	1053.637	1053.642003
7	4	20	5	19	207.829378100	1053.76505	1053.770053
7	3	45	2	46	678.963668100	1053.79477	1053.799773
7	2	36	1	37	428.216200100	1053.80158	1053.806583
7	1	27	0	28	236.835719500	1053.83952	1053.844524
7	0	18	1	19	104.925193700	1053.87771	1053.882714
7	5	27	6	26	355.232706400	1053.87771	1053.882714
7	6	36	7	35	585.928846800	1053.92627	1053.931274
7	1	9	2	10	32.554267720	1054.0064	1054.011404
7	3	8	4	7	66.541567470	1054.2537	1054.258706
7	3	46	2	47	707.138913300	1054.38871	1054.393716
7	4	19	5	18	195.563520100	1054.38871	1054.393716
7	2	37	1	38	450.895065600	1054.39986	1054.404866

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	1	28	0	29	254.007403900	1054.44133	1054.446336
7	0	19	1	20	116.581714400	1054.48006	1054.485067
7	5	26	6	25	338.681140400	1054.49910	1054.504107
7	6	35	7	34	563.875004600	1054.53495	1054.539957
7	1	10	2	11	38.690486480	1054.61045	1054.615457
7	3	7	4	6	61.633202760	1054.8699	1054.874909
7	3	47	2	48	735.924447400	1054.98314	1054.988149
7	2	38	1	39	474.185426500	1054.99793	1055.002939
7	4	18	5	17	183.910580200	1055.00450	1055.009509
7	1	29	0	30	271.791523000	1055.04372	1055.048729
7	0	20	1	21	128.851340000	1055.08192	1055.08693
7	5	25	6	24	322.741899700	1055.11810	1055.12311
7	6	34	7	33	542.432518200	1055.14319	1055.1482
7	1	11	2	12	45.440209780	1055.21924	1055.22425
7	2	2	3	3	21.599875100	1055.3476	1055.352611
7	3	6	4	5	57.338330420	1055.4858	1055.490811
7	3	48	2	49	765.320127200	1055.57695	1055.581962
7	2	39	1	40	498.087167200	1055.59515	1055.600162
7	4	17	5	16	172.870615900	1055.62275	1055.627762
7	1	30	0	31	290.187988400	1055.64408	1055.649092
7	0	21	1	22	141.734009300	1055.7258	1055.730813
7	5	24	6	23	307.415063300	1055.73853	1055.743543
7	6	33	7	32	521.601493300	1055.74930	1055.754313
7	1	12	2	13	52.803404110	1055.82784	1055.832853
7	2	3	3	4	23.440772910	1055.95442	1055.959434
7	3	5	4	4	53.656971740	1056.1013	1056.106314
7	2	40	1	41	522.600168800	1056.19175	1056.196765
7	1	31	0	32	309.196708700	1056.24437	1056.249385
7	4	16	5	15	162.443682000	1056.24437	1056.249385
7	0	22	1	23	155.229658500	1056.28408	1056.289095
7	6	32	7	31	501.382032600	1056.35320	1056.358216

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	1	13	2	14	60.780032900	1056.43598	1056.440996
7	2	4	3	5	25.895289110	1056.56614	1056.571157
7	2	41	1	42	547.724309500	1056.78819	1056.793208
7	1	32	0	33	328.817589400	1056.84499	1056.850008
7	4	15	5	14	152.629830000	1056.8590	1056.864018
7	0	23	1	24	169.338220400	1056.88417	1056.889188
7	6	31	7	30	481.774235900	1056.95840	1056.963418
7	5	22	6	21	278.598902700	1056.97539	1056.980409
7	1	14	2	15	69.370056520	1057.04319	1057.048209
7	2	5	3	6	28.963411520	1057.1824	1057.18742
7	2	42	1	43	573.459464300	1057.38421	1057.38923
7	1	33	0	34	349.050533000	1057.44477	1057.449791
7	4	14	5	13	143.429108500	1057.47020	1057.475221
7	0	24	1	25	184.059624900	1057.48346	1057.488481
7	6	30	7	29	462.778199700	1057.56130	1057.566321
7	5	21	6	20	265.109721000	1057.59492	1057.599941
7	1	15	2	16	78.573432310	1057.65066	1057.655682
7	2	6	3	7	32.645124920	1057.788	1057.793022
7	1	34	0	35	369.895438800	1058.0439	1058.048924
7	0	25	1	26	199.393798800	1058.0824	1058.087424
7	4	13	5	12	134.841563100	1058.09424	1058.099264
7	6	29	7	28	444.394017900	1058.16199	1058.167014
7	5	20	6	19	252.233228100	1058.22029	1058.225314
7	1	16	2	17	88.390114560	1058.25755	1058.262575
7	2	7	3	8	36.940411040	1058.39827	1058.403295
7	3	55	4	55	988.161312800	1058.53813	1058.543156
7	3	54	4	54	954.498873700	1058.56203	1058.567056
7	3	53	4	53	921.445493700	1058.58453	1058.589556
7	3	52	4	52	889.001337200	1058.60658	1058.611606
7	3	51	4	51	857.166565500	1058.62892	1058.633946
7	1	35	0	36	391.352203200	1058.64228	1058.647306

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ (K=6) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground.State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	3	50	4	50	825.941337000	1058.64964	1058.654666
7	3	49	4	49	795.325806800	1058.67051	1058.675537
7	0	26	1	27	215.340666000	1058.68077	1058.685797
7	3	48	4	48	765.320127200	1058.69072	1058.695747
7	3	47	4	47	735.924447400	1058.71069	1058.715717
7	4	12	5	11	126.867236200	1058.71069	1058.715717
7	3	46	4	46	707.138913300	1058.73037	1058.735397
7	3	45	4	45	678.963668100	1058.7492	1058.754227
7	3	44	4	44	651.398851900	1058.76763	1058.772657
7	6	28	7	27	426.621780900	1058.76763	1058.772657
7	3	43	4	43	624.444601400	1058.78586	1058.790887
7	3	42	4	42	598.101050700	1058.80372	1058.808747
7	3	41	4	41	572.368330500	1058.82108	1058.826107
7	5	19	6	18	239.969487600	1058.82890	1058.833927
7	3	40	4	40	547.246568800	1058.83789	1058.842917
7	3	39	4	39	522.735890200	1058.85439	1058.859417
7	1	17	2	18	98.820054490	1058.86321	1058.868237
7	3	38	4	38	498.836416500	1058.87029	1058.875318
7	3	37	4	37	475.548266400	1058.88584	1058.890868
7	3	36	4	36	452.871555400	1058.90095	1058.905978
7	3	35	4	35	430.806396100	1058.91564	1058.920668
7	3	34	4	34	409.352898200	1058.92982	1058.934848
7	3	33	4	33	388.511167900	1058.94376	1058.948788
7	7	40	8	39	744.247818100	1058.94376	1058.948788
7	3	32	4	32	368.281308900	1058.95709	1058.962118
7	3	31	4	31	348.663421400	1058.96997	1058.974998
7	3	30	4	30	329.657602900	1058.98255	1058.987578
7	3	29	4	29	311.263947700	1058.9948	1058.999828
7	2	8	3	9	41.849248560	1059.00715	1059.012178
7	3	27	4	27	276.313488800	1059.01781	1059.022838
7	3	26	4	26	259.756858700	1059.02869	1059.033718

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	3	25	4	25	243.812738500	1059.03917	1059.044198
7	3	24	4	24	228.481207400	1059.04912	1059.054148
7	3	23	4	23	213.762341500	1059.05865	1059.063678
7	3	22	4	22	199.656213800	1059.06791	1059.072938
7	3	21	4	21	186.162894100	1059.07668	1059.081708
7	3	20	4	20	173.282449400	1059.08498	1059.090009
7	3	19	4	19	161.014943600	1059.09305	1059.098079
7	3	18	4	18	149.360437500	1059.10054	1059.105569
7	3	17	4	17	138.318988900	1059.1076	1059.112629
7	3	16	4	16	127.890652600	1059.11425	1059.119279
7	3	15	4	15	118.075480100	1059.12054	1059.125569
7	3	14	4	14	108.873520300	1059.12681	1059.131839
7	1	36	0	37	413.420719500	1059.24138	1059.246409
7	0	27	1	28	231.900147100	1059.27855	1059.283579
7	4	11	5	10	119.506167300	1059.32830	1059.33333
7	6	27	7	26	409.461576300	1059.36162	1059.36665
7	5	18	6	17	228.318560200	1059.44612	1059.45115
7	1	18	2	19	109.863200300	1059.46955	1059.47458
7	7	39	8	38	719.755696500	1059.46955	1059.47458
7	2	9	3	10	47.371613130	1059.61813	1059.623161
7	1	37	0	38	436.100878000	1059.83854	1059.843572
7	0	28	1	29	249.072159800	1059.87518	1059.880212
7	6	26	7	25	392.913488900	1059.95913	1059.964163
7	5	17	6	16	217.280503400	1060.06252	1060.067553
7	1	19	2	20	121.519497200	1060.07486	1060.079893
7	2	10	3	11	53.507477330	1060.22738	1060.232414
7	8	46	9	45	977.771891600	1060.27610	1060.281134
7	1	38	0	39	459.392565800	1060.43599	1060.441025
7	0	29	1	30	266.856618800	1060.47186	1060.476895
7	6	25	7	24	376.977600000	1060.55580	1060.560836
7	1	20	2	21	133.788887100	1060.67927	1060.684306

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	5	16	6	15	206.855371700	1060.67972	1060.684756
7	2	11	3	12	60.256810720	1060.83596	1060.840997
7	8	45	9	44	949.625805200	1060.89720	1060.902237
7	9	54	10	53	1308.333224000	1061.01910	1061.024138
7	1	39	0	40	483.295667000	1061.03238	1061.037418
7	0	30	1	31	285.253435600	1061.06767	1061.072708
7	6	24	7	23	361.653988200	1061.15227	1061.157308
7	1	21	2	22	146.671309200	1061.2843	1061.289339
7	2	12	3	13	67.619579800	1061.4442	1061.44924
7	3	3	4	4	48.134865300	1061.61835	1061.623391
7	1	40	0	41	507.810062800	1061.629	1061.634041
7	0	31	1	32	304.262518800	1061.66278	1061.667821
7	7	35	8	34	627.895940900	1061.7150	1061.720041
7	6	23	7	22	346.942729100	1061.74630	1061.751341
7	1	22	2	23	160.166699500	1061.88845	1061.893492
7	2	13	3	14	75.595748030	1062.05252	1062.057563
7	8	43	9	42	895.163240100	1062.13348	1062.138523
7	1	41	0	42	532.935631300	1062.22991	1062.234953
7	3	4	4	5	50.589144970	1062.22991	1062.234953
7	0	32	1	33	323.883773800	1062.25719	1062.262234
7	9	52	10	51	1242.923690000	1062.28040	1062.285444
7	7	34	8	33	606.458749300	1062.28770	1062.292744
7	6	22	7	21	332.843895000	1062.33951	1062.344554
7	1	23	2	24	174.274990900	1062.49196	1062.497005
7	5	13	6	12	179.258026700	1062.53310	1062.538145
7	2	14	3	15	84.185275820	1062.65952	1062.664566
7	8	42	9	41	868.847028500	1062.74250	1062.747546
7	1	42	0	43	558.672247300	1062.81973	1062.824776
7	3	5	4	6	53.656971740	1062.84098	1062.846026
7	0	33	1	34	344.117103000	1062.85118	1062.856226
7	7	33	8	32	585.632872000	1062.87330	1062.878347

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	6	21	7	20	319.357555600	1062.93340	1062.938447
7	1	24	2	25	188.996113200	1063.09495	1063.099998
7	2	15	3	16	93.388120530	1063.26646	1063.271508
7	8	41	9	40	843.141037300	1063.36250	1063.367549
7	1	43	0	44	585.019782900	1063.4141	1063.419149
7	0	34	1	35	364.962405900	1063.44426	1063.449309
7	3	6	4	7	57.338330420	1063.45181	1063.456859
7	7	32	8	31	565.418411400	1063.46490	1063.469949
7	9	50	10	49	1179.948601000	1063.54740	1063.55245
7	1	25	2	26	204.329993400	1063.69615	1063.7012
7	2	16	3	17	103.204236500	1063.87286	1063.877911
7	1	44	0	45	611.978106800	1064.00813	1064.013182
7	0	35	1	36	386.419578700	1064.03707	1064.042122
7	3	7	4	8	61.633202760	1064.0621	1064.067152
7	6	19	7	18	294.222623100	1064.11593	1064.120982
7	4	55	5	55	1022.600321000	1064.26635	1064.271403
7	1	26	2	27	220.276555300	1064.30001	1064.305063
7	4	51	5	51	891.622721100	1064.35098	1064.356034
7	4	50	5	50	860.401591200	1064.37335	1064.378404
7	4	49	5	49	829.790083900	1064.39313	1064.398184
7	4	48	5	48	799.788351000	1064.41369	1064.418744
7	4	47	5	47	770.396541600	1064.43341	1064.438464
7	5	10	6	9	157.178679000	1064.43341	1064.438464
7	4	46	5	46	741.614801400	1064.4522	1064.457254
7	4	45	5	45	713.443273200	1064.47122	1064.476274
7	2	17	3	18	113.633575000	1064.47891	1064.483964
7	4	44	5	44	685.882096800	1064.4893	1064.494354
7	4	43	5	43	658.931408900	1064.50753	1064.512584
7	4	42	5	42	632.591343200	1064.52555	1064.530604
7	4	41	5	41	606.862030300	1064.54125	1064.546304
7	4	40	5	40	581.743597700	1064.55834	1064.563395

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	4	39	5	39	557.236170200	1064.57363	1064.578685
7	4	38	5	38	533.339869000	1064.58925	1064.594305
7	1	45	0	46	639.547085000	1064.6041	1064.609155
7	4	37	5	37	510.054812700	1064.6041	1064.609155
7	8	39	9	38	793.560217300	1064.60410	1064.609155
7	4	36	5	36	487.381116800	1064.61925	1064.624305
7	0	36	1	37	408.488514800	1064.63011	1064.635165
7	4	34	5	34	443.868252300	1064.64688	1064.651935
7	7	30	8	29	526.824134500	1064.64688	1064.651935
7	4	33	5	33	423.029299300	1064.66005	1064.665105
7	3	8	4	9	66.541567470	1064.67222	1064.677275
7	4	31	5	31	383.186868300	1064.6852	1064.690255
7	4	30	5	30	364.183587600	1064.69684	1064.701895
7	4	29	5	29	345.792390000	1064.70856	1064.713615
7	6	18	7	17	282.574153800	1064.70856	1064.713615
7	4	28	5	28	328.013366600	1064.71935	1064.724405
7	4	27	5	27	310.846605400	1064.72991	1064.734965
7	4	26	5	26	294.292191500	1064.7398	1064.744855
7	4	25	5	25	278.350206800	1064.7496	1064.754655
7	4	24	5	24	263.020730200	1064.75868	1064.763735
7	4	23	5	23	248.303837700	1064.76771	1064.772766
7	4	22	5	22	234.199602100	1064.77603	1064.781086
7	4	21	5	21	220.708093300	1064.78408	1064.789136
7	4	20	5	20	207.829378100	1064.79171	1064.796766
7	4	19	5	19	195.563520100	1064.79878	1064.803836
7	4	18	5	18	183.910580200	1064.80506	1064.810116
7	9	48	10	47	1119.409190000	1064.80506	1064.810116
7	4	17	5	17	172.870615900	1064.81177	1064.816826
7	1	27	2	28	236.835719500	1064.9019	1064.906956
7	5	9	6	8	151.045294800	1065.00340	1065.008457
7	2	18	3	19	124.676084300	1065.08457	1065.089627

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground.State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	1	46	0	47	667.726580300	1065.19491	1065.199968
7	0	37	1	38	431.169104300	1065.22014	1065.225198
7	7	29	8	28	508.444507900	1065.25030	1065.255358
7	3	9	4	10	72.063400220	1065.28159	1065.286648
7	6	17	7	16	271.538426800	1065.29943	1065.304488
7	1	28	2	29	254.007403900	1065.50289	1065.507949
7	2	19	3	20	136.331709500	1065.68967	1065.69473
7	0	38	1	39	454.461234400	1065.81074	1065.8158
7	7	28	8	27	490.676677300	1065.85064	1065.855701
7	8	37	9	36	746.421752200	1065.85064	1065.855701
7	3	10	4	11	78.198673650	1065.8906	1065.895661
7	6	16	7	15	261.115496300	1065.89060	1065.895661
7	1	29	2	30	271.791523000	1066.10363	1066.108692
7	5	7	6	6	140.618309900	1066.21860	1066.223662
7	2	20	3	21	148.600392700	1066.29447	1066.299533
7	0	39	1	40	478.364789200	1066.40055	1066.405613
7	3	11	4	12	84.947357350	1066.4992	1066.504264
7	1	30	2	31	290.187988400	1066.70407	1066.709135
7	2	21	3	22	161.482073200	1066.89874	1066.903806
7	0	40	1	41	502.879649900	1066.98983	1066.994896
7	3	12	4	13	92.309417860	1067.1075	1067.112567
7	1	31	2	32	309.196708700	1067.3034	1067.308468
7	2	22	3	23	174.976686900	1067.50248	1067.507549
7	0	41	1	42	528.005694300	1067.57848	1067.583549
7	6	13	7	12	233.523982200	1067.66619	1067.671259
7	7	25	8	24	441.044819400	1067.66619	1067.671259
7	3	13	4	14	100.284818700	1067.7153	1067.72037
7	8	34	9	33	680.295478700	1067.71530	1067.72037
7	1	32	2	33	328.817589400	1067.90367	1067.90874
7	4	4	5	5	85.152586000	1067.92352	1067.928591
7	9	43	10	42	978.724402600	1067.95470	1067.959771

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground.State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	2	23	3	24	189.084166700	1068.106	1068.111071
7	0	42	1	43	553.742797400	1068.16661	1068.171682
7	7	24	8	23	425.725015600	1068.27590	1068.280972
7	3	14	4	15	108.873520300	1068.3226	1068.327672
7	1	33	2	34	349.050533000	1068.50202	1068.507093
7	4	5	5	6	88.219999040	1068.535	1068.540073
7	2	24	3	25	203.804442800	1068.70875	1068.713824
7	0	43	1	44	580.090831200	1068.75395	1068.759024
7	7	23	8	22	411.017414100	1068.8840	1068.889075
7	3	15	4	16	118.075480100	1068.9293	1068.934375
7	8	32	9	31	639.266838900	1068.97250	1068.977575
7	1	34	2	35	369.895438800	1069.10056	1069.105636
7	4	6	5	7	91.900861300	1069.14564	1069.150716
7	2	25	3	26	219.137441900	1069.31099	1069.316067
7	0	44	1	45	607.049664500	1069.34086	1069.345937
7	6	10	7	9	211.449303600	1069.450	1069.455078
7	3	16	4	17	127.890652600	1069.5359	1069.540978
7	8	31	9	30	619.669487700	1069.58423	1069.589308
7	1	35	2	36	391.352203200	1069.69824	1069.703319
7	4	7	5	8	96.195154570	1069.75599	1069.761069
7	9	40	10	39	901.631280800	1069.84220	1069.84728
7	2	26	3	27	235.083088000	1069.91257	1069.91765
7	0	45	1	46	634.619163100	1069.92603	1069.93111
7	6	9	7	8	205.317217000	1070.04773	1070.052811
7	3	17	4	18	138.318988900	1070.1418	1070.146881
7	5	46	6	46	785.927361300	1070.16847	1070.173551
7	5	45	6	45	757.760609600	1070.1874	1070.192481
7	5	44	6	44	730.204110600	1070.20503	1070.210111
7	8	30	9	29	600.683577900	1070.20503	1070.210111
7	5	43	6	43	703.258000800	1070.22184	1070.226921
7	5	42	6	42	676.922413400	1070.23876	1070.243841

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	5	41	6	41	651.197478900	1070.25494	1070.260022
7	5	40	6	40	626.083324600	1070.2701	1070.275182
7	5	39	6	39	601.580074700	1070.28498	1070.290062
7	1	36	2	37	413.420719500	1070.29727	1070.302352
7	5	38	6	38	577.687850400	1070.29727	1070.302352
7	5	37	6	37	554.406769900	1070.31314	1070.318222
7	5	36	6	36	531.736948400	1070.32657	1070.331652
7	5	35	6	35	509.678498000	1070.33922	1070.344302
7	5	34	6	34	488.231527700	1070.3516	1070.356682
7	4	8	5	9	101.102857600	1070.36561	1070.370692
7	5	33	6	33	467.396143700	1070.36561	1070.370692
7	5	32	6	32	447.172448800	1070.37556	1070.380642
7	5	31	6	31	427.560543200	1070.38515	1070.390232
7	5	30	6	30	408.560523800	1070.39504	1070.400122
7	5	29	6	29	390.172484400	1070.40486	1070.409942
7	5	28	6	28	372.396516000	1070.41367	1070.418752
7	5	27	6	27	355.232706400	1070.42237	1070.427452
7	5	26	6	26	338.681140400	1070.43067	1070.435752
7	5	25	6	25	322.741899700	1070.43863	1070.443712
7	5	24	6	24	307.415063300	1070.44593	1070.451012
7	5	23	6	23	292.700706700	1070.45251	1070.457593
7	5	22	6	22	278.598902700	1070.45859	1070.463673
7	2	27	3	28	251.641301800	1070.50964	1070.514723
7	3	18	4	19	149.360437500	1070.7473	1070.752384
7	1	37	2	38	436.100878000	1070.89269	1070.897775
7	4	9	5	10	106.623946100	1070.97651	1070.981595
7	0	47	1	48	691.589604100	1071.09599	1071.101076
7	2	28	3	29	268.812001100	1071.1146	1071.119686
7	3	19	4	20	161.014943600	1071.3524	1071.357487
7	1	38	2	39	459.392565800	1071.48881	1071.493897
7	4	10	5	11	112.758392800	1071.58542	1071.590508

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground.State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	0	48	1	49	720.990262900	1071.67988	1071.684968
7	2	29	3	30	286.595100700	1071.71504	1071.720129
7	3	20	4	21	173.282449400	1071.9569	1071.96199
7	1	39	2	40	483.295667000	1072.08431	1072.0894
7	4	11	5	12	119.506167300	1072.19435	1072.199441
7	0	49	1	50	751.001019500	1072.26237	1072.267461
7	2	30	3	31	304.990512100	1072.31515	1072.320241
7	3	21	4	22	186.162894100	1072.5609	1072.565993
7	7	17	8	16	335.631889200	1072.56094	1072.566033
7	1	40	2	41	507.810062800	1072.67981	1072.684903
7	8	26	9	25	530.856167500	1072.69920	1072.704293
7	4	12	5	13	126.867236200	1072.80273	1072.807824
7	0	50	1	51	781.621724600	1072.84517	1072.850264
7	2	31	3	32	323.998144100	1072.91423	1072.919324
7	3	22	4	23	199.656213800	1073.1648	1073.169895
7	7	16	8	15	325.211558000	1073.16481	1073.169905
7	1	41	2	42	532.935631300	1073.27426	1073.279356
7	8	25	9	24	514.928799300	1073.32170	1073.326796
7	4	13	5	14	134.841563100	1073.41082	1073.415917
7	0	51	1	52	812.852225600	1073.42628	1073.431377
7	2	32	3	33	343.617902200	1073.51364	1073.518737
7	3	23	4	24	213.762341500	1073.7678	1073.772898
7	1	42	2	43	558.672247300	1073.86839	1073.873489
7	0	52	1	53	844.692367000	1074.00767	1074.012769
7	4	14	5	15	143.429108500	1074.01828	1074.023379
7	2	33	3	34	363.849688800	1074.11176	1074.11686
7	5	5	6	6	132.644536400	1074.1941	1074.1992
7	9	33	10	32	743.112470800	1074.24449	1074.249591
7	3	24	4	25	228.481207400	1074.3703	1074.375401
7	1	43	2	44	585.019782900	1074.46269	1074.467792
7	8	23	9	22	484.910000400	1074.56347	1074.568572

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	0	53	1	54	877.141990000	1074.58796	1074.593062
7	4	15	5	16	152.629830000	1074.62574	1074.630842
7	2	34	3	35	384.693403600	1074.70951	1074.714613
7	5	6	6	7	136.324760700	1074.8083	1074.813403
7	3	25	4	26	243.812738500	1074.9725	1074.977604
7	1	44	2	45	611.978106800	1075.05575	1075.060854
7	0	54	1	55	910.200933100	1075.16729	1075.172395
7	4	16	5	17	162.443682000	1075.23236	1075.237465
7	2	35	3	36	406.148942900	1075.30688	1075.311986
7	5	7	6	8	140.618309900	1075.4182	1075.423306
7	9	31	10	30	703.319281100	1075.49647	1075.501576
7	3	26	4	27	259.756858700	1075.5743	1075.579407
7	6	9	7	9	205.317217000	1075.58319	1075.588297
7	6	10	7	10	211.449303600	1075.60108	1075.606187
7	6	11	7	11	218.194482700	1075.61945	1075.624557
7	6	12	7	12	225.552720900	1075.63893	1075.644037
7	1	45	2	46	639.547085000	1075.65862	1075.663727
7	6	13	7	13	233.523982200	1075.65862	1075.663727
7	6	14	7	14	242.108227200	1075.68	1075.685107
7	6	15	7	15	251.305413600	1075.7011	1075.706207
7	6	16	7	16	261.115496300	1075.72239	1075.727498
7	6	17	7	17	271.538426800	1075.74414	1075.749248
7	6	18	7	18	282.574153800	1075.76501	1075.770118
7	6	19	7	19	294.222623100	1075.7857	1075.790808
7	6	20	7	20	306.483777100	1075.80622	1075.811328
7	8	21	9	20	457.339602800	1075.80622	1075.811328
7	6	21	7	21	319.357555600	1075.82594	1075.831048
7	4	17	5	18	172.870615900	1075.83826	1075.843368
7	6	22	7	22	332.843895000	1075.84465	1075.849758
7	6	23	7	23	346.942729100	1075.86266	1075.867768
7	6	24	7	24	361.653988200	1075.87963	1075.884738

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	6	25	7	25	376.977600000	1075.8986	1075.903708
7	2	36	3	37	428.216200100	1075.90379	1075.908898
7	6	49	7	49	928.208544700	1075.90379	1075.908898
7	6	26	7	26	392.913488900	1075.9133	1075.918408
7	6	47	7	47	868.837317300	1075.91568	1075.920788
7	6	27	7	27	409.461576300	1075.92285	1075.927958
7	6	28	7	28	426.621780900	1075.93518	1075.940289
7	6	29	7	29	444.394017900	1075.94582	1075.950929
7	6	30	7	30	462.778199700	1075.9589	1075.964009
7	6	31	7	31	481.774235900	1075.9670	1075.972109
7	5	8	6	9	145.525162600	1076.0928	1076.097909
7	3	27	4	28	276.313488800	1076.1754	1076.18051
7	1	46	2	47	667.726580300	1076.24057	1076.24568
7	7	11	8	10	282.301258500	1076.24057	1076.24568
7	4	18	5	19	183.910580200	1076.44452	1076.449631
7	2	37	3	38	450.895065600	1076.49959	1076.504701
7	5	9	6	10	151.045294800	1076.6413	1076.646412
7	9	29	10	28	665.971080200	1076.74820	1076.753312
7	3	28	4	29	293.482546900	1076.7761	1076.781213
7	1	47	2	48	696.516452200	1076.83235	1076.837463
7	4	19	5	20	195.563520100	1077.04983	1077.054944
7	8	19	9	18	432.218146000	1077.04983	1077.054944
7	2	38	3	39	474.185426500	1077.09547	1077.100584
7	5	10	6	11	157.178679000	1077.25318	1077.258295
7	3	29	4	30	311.263947700	1077.3758	1077.380915
7	9	28	10	27	648.214080100	1077.37588	1077.380995
7	1	48	2	49	725.916557600	1077.42311	1077.428226
7	4	20	5	21	207.829378100	1077.65497	1077.660087
7	2	39	3	40	498.087167200	1077.69067	1077.695787
7	5	11	6	12	163.925285200	1077.86568	1077.870798
7	3	30	4	31	329.657602900	1077.9756	1077.980718

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ (K=6) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground.State Energy (cm ⁻¹)	Transition Energy (cm ⁻¹)	Calibrated Transition Energy (cm ⁻¹)
7	1	49	2	50	755.926750000	1078.0129	1078.018018
7	4	21	5	22	220.708093300	1078.25894	1078.26406
7	2	40	3	41	522.600168800	1078.28527	1078.29039
7	8	17	9	16	409.546121600	1078.28527	1078.29039
3 ν_8	6	8	7	8	199.798253000	1078.30093	1078.30605
3 ν_8	6	10	7	10	211.449303600	1078.32492	1078.33004
3 ν_8	6	7	7	7	194.892438800	1078.43058	1078.4357
3 ν_8	6	9	7	9	205.317217000	1078.454406	1078.459527
3 ν_8	6	11	7	11	218.194482700	1078.482696	1078.487817
7	5	12	6	13	171.285079800	1078.48382	1078.488941
3 ν_8	6	12	7	12	225.552720900	1078.51406	1078.519181
7	3	31	4	32	348.663421400	1078.5749	1078.580021
3 ν_8	6	13	7	13	233.523982200	1078.57498	1078.580101
3 ν_8	6	14	7	14	242.108227200	1078.58848	1078.593601
3 ν_8	6	15	7	15	251.305413600	1078.60367	1078.608791
7	1	50	2	51	786.546879900	1078.60367	1078.608791
3 ν_8	6	16	7	16	261.115496300	1078.63125	1078.636371
3 ν_8	6	17	7	17	271.538426800	1078.67897	1078.684092
3 ν_8	6	18	7	18	282.574153800	1078.85054	1078.855662
3 ν_8	6	19	7	19	294.222623100	1078.86253	1078.867652
7	4	22	5	23	234.199602100	1078.86253	1078.867652
3 ν_8	6	20	7	20	306.483777100	1078.87984	1078.884963
7	2	41	3	42	547.724309500	1078.87984	1078.884963
7	8	16	9	15	399.128787000	1078.90720	1078.912323
3 ν_8	6	21	7	21	319.357555600	1078.98985	1078.994973
7	5	13	6	14	179.258026700	1079.07567	1079.080793
3 ν_8	6	22	7	22	332.843895000	1079.151	1079.156124
7	3	32	4	33	368.281308900	1079.1735	1079.178624
3 ν_8	6	23	7	23	346.942729100	1079.17359	1079.178714
7	1	51	2	52	817.776795000	1079.19322	1079.198344
7	4	23	5	24	248.303837700	1079.46627	1079.471395

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	2	42	3	43	573.459464300	1079.47271	1079.477835
7	5	14	6	15	187.844086400	1079.68899	1079.694116
7	3	33	4	34	388.511167900	1079.7714	1079.776527
7	6	6	7	7	190.599798500	1079.84519	1079.850317
7	2	43	3	44	599.805505300	1080.06811	1080.073238
7	5	15	6	16	197.043216500	1080.29869	1080.303819
7	3	34	4	35	409.352898200	1080.3692	1080.37433
7	6	7	7	8	194.892438800	1080.47315	1080.47828
7	2	44	3	45	626.762301500	1080.65877	1080.663901
7	4	25	5	26	278.350206800	1080.67145	1080.676581
7	5	16	6	17	206.855371700	1080.90889	1080.914022
7	3	35	4	36	430.806396100	1080.9659	1080.971032
7	6	8	7	9	199.798253000	1081.1024	1081.107533
7	2	45	3	46	654.329718700	1081.25098	1081.256114
7	4	26	5	27	294.292191500	1081.27378	1081.278914
7	5	17	6	18	217.280503400	1081.51742	1081.522555
7	3	36	4	37	452.871555400	1081.5624	1081.567535
7	6	9	7	10	205.317217000	1081.733	1081.738136
7	2	46	3	47	682.507619900	1081.84211	1081.847247
7	4	27	5	28	310.846605400	1081.87491	1081.880047
7	5	18	6	19	228.318560200	1082.12575	1082.130888
7	3	37	4	38	475.548266400	1082.1582	1082.163338
7	6	10	7	11	211.449303600	1082.36468	1082.369819
7	9	20	10	19	528.179321100	1082.36468	1082.369819
$3\nu_8$	6	6	7	7	190.599798500	1082.43211	1082.437249
7	4	28	5	29	328.013366600	1082.47569	1082.48083
7	5	19	6	20	239.969487600	1082.72322	1082.728361
7	3	38	4	39	498.836416500	1082.7533	1082.758441
7	6	11	7	12	218.194482700	1082.99754	1083.002682
7	7	26	8	26	456.976750300	1082.99754	1083.002682
7	7	27	8	27	473.520730000	1083.00642	1083.011562

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ (K=6) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	2	48	3	49	740.694310400	1083.01676	1083.021902
7	7	29	8	29	508.444507900	1083.03067	1083.035812
7	7	30	8	30	526.824134500	1083.04719	1083.052332
7	7	31	8	31	545.815466800	1083.06608	1083.071222
7	4	29	5	30	345.792390000	1083.07613	1083.081272
7	7	32	8	32	565.418411400	1083.08948	1083.094623
7	7	33	8	33	585.632872000	1083.11766	1083.122803
7	7	35	8	35	627.895940900	1083.19144	1083.196583
$3\nu_8$	6	7	7	8	194.892438800	1083.29382	1083.298963
7	7	37	8	37	672.603842100	1083.29382	1083.298963
7	5	20	6	21	252.233228100	1083.34089	1083.346034
7	3	39	4	40	522.735890200	1083.3483	1083.353444
7	7	38	8	38	695.874332000	1083.36022	1083.365364
7	7	40	8	40	744.247818100	1083.52469	1083.529835
7	2	49	3	50	770.702810200	1083.6124	1083.617545
7	9	18	10	17	504.290296600	1083.61240	1083.617545
7	6	12	7	13	225.552720900	1083.63008	1083.635225
7	4	30	5	31	364.183587600	1083.67604	1083.681185
$3\nu_8$	6	8	7	9	199.798253000	1083.78835	1083.793496
7	3	40	4	41	547.246568800	1083.9431	1083.948247
7	5	21	6	22	265.109721000	1083.949	1083.954147
7	2	50	3	51	801.321215000	1084.2011	1084.206248
7	6	13	7	14	233.523982200	1084.26392	1084.269068
7	4	31	5	32	383.186868300	1084.27497	1084.280118
7	3	41	4	42	572.368330500	1084.5362	1084.541349
$3\nu_8$	6	9	7	10	205.317217000	1084.53629	1084.541439
7	5	22	6	23	278.598902700	1084.55406	1084.559209
7	2	51	3	52	832.549372300	1084.79014	1084.795291
7	4	32	5	33	402.802137900	1084.87406	1084.879211
7	6	14	7	15	242.108227200	1084.89826	1084.903411
7	3	42	4	43	598.101050700	1085.1294	1085.134552

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ (K=6) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
$3\nu_8$	6	10	7	11	211.449303600	1085.12943	1085.134582
7	5	23	6	24	292.700706700	1085.15966	1085.164812
7	4	33	5	34	423.029299300	1085.47198	1085.477134
7	9	15	10	14	473.048521100	1085.47198	1085.477134
7	6	15	7	16	251.305413600	1085.53241	1085.537564
7	3	43	4	44	624.444601400	1085.7218	1085.726955
$3\nu_8$	6	11	7	12	218.194482700	1085.72186	1085.727015
7	5	24	6	25	307.415063300	1085.76498	1085.770135
7	4	34	5	35	443.868252300	1086.06967	1086.074827
7	6	16	7	17	261.115496300	1086.16653	1086.171687
7	3	44	4	45	651.398851900	1086.3138	1086.318958
$3\nu_8$	6	12	7	13	225.552720900	1086.35178	1086.356938
7	5	25	6	26	322.741899700	1086.36953	1086.374688
7	10	34	11	33	857.330121900	1086.36953	1086.374688
7	11	33	12	32	939.689763600	1086.36953	1086.374688
7	4	35	5	36	465.318893500	1086.66656	1086.671719
7	6	17	7	18	271.538426800	1086.80055	1086.80571
7	3	45	4	46	678.963668100	1086.9051	1086.910261
$3\nu_8$	6	13	7	14	233.523982200	1086.97364	1086.978801
7	5	26	6	27	338.681140400	1086.97364	1086.978801
7	4	36	5	37	487.381116800	1087.26309	1087.268252
7	6	18	7	19	282.574153800	1087.43421	1087.439373
7	3	46	4	47	707.138913300	1087.4959	1087.501063
7	5	27	6	28	355.232706400	1087.57761	1087.582774
$3\nu_8$	6	14	7	15	242.108227200	1087.80915	1087.814315
7	4	37	5	38	510.054812700	1087.85899	1087.864155
7	7	7	8	8	259.005038100	1087.88753	1087.892695
7	6	19	7	20	294.222623100	1088.06757	1088.072736
7	3	47	4	48	735.924447400	1088.086	1088.091166
7	5	28	6	29	372.396516000	1088.18063	1088.185797
7	8	45	9	45	949.625805200	1088.41871	1088.423878

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	4	38	5	39	533.339869000	1088.45457	1088.459738
7	8	40	9	40	818.045392600	1088.45457	1088.459738
7	8	39	9	39	793.560217300	1088.46817	1088.473338
7	8	38	9	38	769.685631500	1088.4779	1088.483068
7	8	37	9	37	746.421752200	1088.4907	1088.495868
7	7	8	8	9	263.909625900	1088.49966	1088.504828
7	8	36	9	36	723.768693500	1088.49966	1088.504828
7	8	35	9	35	701.726566300	1088.51281	1088.517978
7	8	34	9	34	680.295478700	1088.52527	1088.530438
7	8	33	9	33	659.475535500	1088.5366	1088.541768
$3\nu_8$	6	15	7	16	251.305413600	1088.54826	1088.553428
7	8	32	9	32	639.266838900	1088.54826	1088.553428
7	8	30	9	30	600.683577900	1088.5713	1088.576469
7	8	29	9	29	582.309202600	1088.58252	1088.587689
7	8	28	9	28	564.546451600	1088.59698	1088.602149
7	8	27	9	27	547.395411900	1088.60576	1088.610929
7	8	26	9	26	530.856167500	1088.61556	1088.620729
7	8	25	9	25	514.928799300	1088.62591	1088.631079
7	8	24	9	24	499.613385300	1088.63648	1088.641649
7	8	23	9	23	484.910000400	1088.64676	1088.651929
7	8	22	9	22	470.818716600	1088.65573	1088.660899
7	8	21	9	21	457.339602800	1088.66481	1088.669979
7	3	48	4	49	765.320127200	1088.6751	1088.680269
7	8	20	9	20	444.472724900	1088.67513	1088.680299
7	8	19	9	19	432.218146000	1088.68246	1088.687629
7	6	20	7	21	306.483777100	1088.69928	1088.704449
7	8	17	9	17	409.546121600	1088.69928	1088.704449
7	8	18	9	18	420.575925900	1088.69928	1088.704449
7	8	10	9	10	349.489287300	1088.74091	1088.746079
7	5	29	6	30	390.172484400	1088.78316	1088.78833
$3\nu_8$	6	16	7	17	261.115496300	1089.04893	1089.054101

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ (K=6) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	4	39	5	40	557.236170200	1089.04893	1089.054101
7	7	9	8	10	269.427210400	1089.11107	1089.116241
7	3	49	4	50	795.325806800	1089.2735	1089.278672
7	6	21	7	22	319.357555600	1089.33101	1089.336182
7	5	30	6	31	408.560523800	1089.3849	1089.390072
7	4	40	5	41	581.743597700	1089.64227	1089.647444
$3\nu_8$	6	17	7	18	271.538426800	1089.7228	1089.727974
7	7	10	8	11	275.557764700	1089.7228	1089.727974
7	3	50	4	51	825.941337000	1089.8794	1089.884575
7	6	22	7	23	332.843895000	1089.96147	1089.966645
7	5	31	6	32	427.560543200	1089.98622	1089.991395
7	4	41	5	42	606.862030300	1090.23681	1090.241986
7	7	11	8	12	282.301258500	1090.3345	1090.339677
$3\nu_8$	6	18	7	19	282.574153800	1090.44123	1090.446407
7	5	32	6	33	447.172448800	1090.58959	1090.594768
7	6	23	7	24	346.942729100	1090.58959	1090.594768
7	10	27	11	26	724.520988300	1090.76016	1090.765339
7	11	26	12	25	811.209728900	1090.76016	1090.765339
7	4	42	5	43	632.591343200	1090.82922	1090.834399
7	7	12	8	13	289.657658900	1090.9464	1090.95158
$3\nu_8$	6	19	7	20	294.222623100	1091.02838	1091.03356
7	5	33	6	34	467.396143700	1091.18708	1091.192261
7	6	24	7	25	361.653988200	1091.21864	1091.223821
7	10	26	11	25	707.993089700	1091.37680	1091.381982
7	11	25	12	24	795.299657900	1091.37680	1091.381982
7	4	43	5	44	658.931408900	1091.42181	1091.426992
7	7	13	8	14	297.626929600	1091.5582	1091.563383
7	5	34	6	35	488.231527700	1091.78641	1091.791594
$3\nu_8$	6	20	7	21	306.483777100	1091.84549	1091.850674
7	6	25	7	26	376.977600000	1091.84549	1091.850674
7	4	44	5	45	685.882096800	1092.01386	1092.019045

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ (K=6) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	7	14	8	15	306.209031600	1092.1704	1092.175586
$3\nu_8$	6	21	7	22	319.357555600	1092.38504	1092.390227
7	5	35	6	36	509.678498000	1092.38504	1092.390227
7	6	26	7	27	392.913488900	1092.47113	1092.476317
7	4	45	5	46	713.443273200	1092.60515	1092.610338
7	7	15	8	16	315.403922800	1092.7822	1092.787389
7	5	36	6	37	531.736948400	1092.98298	1092.988169
7	6	27	7	28	409.461576300	1093.095	1093.10019
7	4	46	5	47	741.614801400	1093.19477	1093.19996
$3\nu_8$	6	22	7	23	332.843895000	1093.34606	1093.351251
7	7	16	8	17	325.211558000	1093.3945	1093.399691
7	5	37	6	38	554.406769900	1093.58072	1093.585912
7	6	28	7	29	426.621780900	1093.71763	1093.722823
7	4	47	5	48	770.396541600	1093.78408	1093.789273
7	7	17	8	18	335.631889200	1094.007	1094.012194
7	9	51	10	51	1211.131762000	1094.07349	1094.078685
7	9	50	10	50	1179.948601000	1094.09575	1094.100945
7	9	49	10	49	1149.374361000	1094.11623	1094.121425
7	5	38	6	39	577.687850400	1094.1781	1094.183295
7	9	46	10	46	1061.306640000	1094.1781	1094.183295
7	8	8	9	9	337.844505200	1094.26126	1094.266456
7	9	42	10	42	952.416621300	1094.26126	1094.266456
7	9	41	10	41	926.718872200	1094.28284	1094.288036
7	9	40	10	40	901.631280800	1094.30195	1094.307146
7	9	39	10	39	877.153969800	1094.32061	1094.325806
7	6	29	7	30	444.394017900	1094.33888	1094.344076
7	9	38	10	38	853.287058400	1094.33888	1094.344076
7	9	37	10	37	830.030663300	1094.35842	1094.363616
7	4	48	5	49	799.788351000	1094.37582	1094.381016
7	9	36	10	36	807.384898000	1094.37582	1094.381016
7	9	35	10	35	785.349873000	1094.39437	1094.399566

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	9	34	10	34	763.925695700	1094.41173	1094.416926
7	9	33	10	33	743.112470800	1094.42902	1094.434216
7	9	32	10	32	722.910299800	1094.44502	1094.450216
7	9	31	10	31	703.319281100	1094.462	1094.467197
7	9	30	10	30	684.339510400	1094.47647	1094.481667
7	9	29	10	29	665.971080200	1094.49175	1094.496947
7	9	28	10	28	648.214080100	1094.50599	1094.511187
7	10	21	11	20	634.527035100	1094.50599	1094.511187
7	11	20	12	19	724.920213800	1094.50599	1094.511187
7	9	27	10	27	631.068596500	1094.52066	1094.525857
7	9	26	10	26	614.534713200	1094.53381	1094.539007
7	9	25	10	25	598.612510600	1094.54776	1094.552957
7	9	24	10	24	583.302066500	1094.56022	1094.565417
7	9	23	10	23	568.603455300	1094.5722	1094.577397
7	9	22	10	22	554.516748800	1094.58447	1094.589667
7	9	21	10	21	541.042015500	1094.59558	1094.600777
7	9	20	10	20	528.179321100	1094.60628	1094.611477
7	7	18	8	19	346.664865000	1094.6187	1094.623897
7	9	19	10	19	515.928728200	1094.61876	1094.623957
7	9	18	10	18	504.290296600	1094.62585	1094.631047
7	9	17	10	17	493.264082900	1094.63545	1094.640647
7	9	16	10	16	482.850140900	1094.64408	1094.649277
7	9	14	10	14	463.859271500	1094.661	1094.666197
7	5	39	6	40	601.580074700	1094.77336	1094.778558
7	8	9	9	10	343.360499600	1094.86898	1094.874178
7	6	30	7	31	462.778199700	1094.95825	1094.963449
7	10	20	11	19	621.669010800	1095.12160	1095.1268
7	11	19	12	18	712.678982400	1095.12160	1095.1268
7	7	19	8	20	358.310431400	1095.2336	1095.2388
7	5	40	6	41	626.083324600	1095.3683	1095.373501
7	8	10	9	11	349.489287300	1095.47708	1095.482281

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	6	31	7	32	481.774235900	1095.57638	1095.581582
7	7	20	8	21	370.568531200	1095.8472	1095.852403
7	5	41	6	42	651.197478900	1095.96292	1095.968124
7	8	11	9	12	356.230838500	1096.08442	1096.089624
7	6	32	7	33	501.382032600	1096.19318	1096.198385
7	7	21	8	22	383.439104300	1096.4618	1096.467006
7	5	42	6	43	676.922413400	1096.55732	1096.562526
7	8	12	9	13	363.585120100	1096.69143	1096.696637
7	6	33	7	34	521.601493300	1096.80866	1096.813868
7	7	22	8	23	396.922087300	1097.0765	1097.081709
7	5	43	6	44	703.258000800	1097.15042	1097.155629
7	8	13	9	14	371.552096200	1097.29799	1097.3032
7	6	34	7	35	542.432518200	1097.4225	1097.427711
7	7	23	8	24	411.017414100	1097.6936	1097.698812
7	5	44	6	45	730.204110600	1097.74334	1097.748552
7	8	14	9	15	380.131727900	1097.90377	1097.908983
7	6	35	7	36	563.875004600	1098.03565	1098.040863
7	7	24	8	25	425.725015600	1098.3108	1098.316015
7	5	45	6	46	757.760609600	1098.33601	1098.341225
7	8	15	9	16	389.323973100	1098.51003	1098.515246
7	6	36	7	37	585.928846800	1098.64847	1098.653686
7	7	25	8	26	441.044819400	1098.9292	1098.934418
7	8	16	9	17	399.128787000	1099.115	1099.120219
7	6	37	7	38	608.593936000	1099.263	1099.268219
7	7	26	8	27	456.976750300	1099.5504	1099.555621
7	8	17	9	18	409.546121600	1099.71949	1099.724711
7	6	38	7	39	631.870160400	1099.89441	1099.899632
7	12	21	13	20	850.756309900	1100.12240	1100.127623
7	7	27	8	28	473.520730000	1100.1733	1100.178524
7	8	18	9	19	420.575925900	1100.32405	1100.329274
7	6	39	7	40	655.757405100	1100.44429	1100.449515

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ (K=6) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	12	20	13	19	837.909078000	1100.75420	1100.759426
7	7	28	8	29	490.676677300	1100.7983	1100.803527
7	9	9	10	10	427.100035800	1100.81335	1100.818577
7	8	19	9	20	432.218146000	1100.92776	1100.932987
7	6	40	7	41	680.255552400	1101.0619	1101.067128
7	9	10	10	11	433.226823700	1101.42014	1101.42537
7	7	29	8	30	508.444507900	1101.4274	1101.43263
7	8	20	9	21	444.472724900	1101.53133	1101.53656
7	6	41	7	42	705.364481300	1101.6702	1101.675431
7	9	11	10	12	439.966175400	1102.02639	1102.031622
7	7	30	8	31	526.824134500	1102.0569	1102.062133
7	8	21	9	22	457.339602800	1102.13447	1102.139703
7	6	42	7	43	731.084067900	1102.27531	1102.280544
7	9	12	10	13	447.318058400	1102.63205	1102.637285
7	7	31	8	32	545.815466800	1102.6921	1102.697336
7	8	22	9	23	470.818716600	1102.73731	1102.742546
7	6	43	7	44	757.414185200	1102.87888	1102.884116
7	9	13	10	14	455.282436600	1103.23716	1103.242398
7	12	16	13	15	792.634444100	1103.23716	1103.242398
7	7	32	8	33	565.418411400	1103.3318	1103.337039
7	8	23	9	24	484.910000400	1103.33932	1103.344559
7	6	44	7	45	784.354703400	1103.48119	1103.486429
7	9	14	10	15	463.859271500	1103.84212	1103.847361
7	8	24	9	25	499.613385300	1103.94179	1103.947032
7	7	33	8	34	585.632872000	1103.977	1103.982242
7	6	45	7	46	811.905489300	1104.0841	1104.089342
7	9	15	10	16	473.048521100	1104.44628	1104.451524
7	8	25	9	26	514.928799300	1104.54255	1104.547794
7	7	34	8	35	606.458749300	1104.6279	1104.633145
7	6	46	7	47	840.066407000	1104.68668	1104.691925
7	9	16	10	17	482.850140900	1105.04981	1105.055057

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ (K=6) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	8	26	9	27	530.856167500	1105.14421	1105.149457
7	6	47	7	48	868.837317300	1105.2881	1105.293348
7	9	17	10	18	493.264082900	1105.65279	1105.65804
7	8	27	9	28	547.395411900	1105.74499	1105.75024
7	6	48	7	49	898.218078300	1105.89433	1105.899581
7	7	36	8	37	649.944341300	1105.9537	1105.958951
7	9	18	10	19	504.290296600	1106.25523	1106.260482
7	8	28	9	29	564.546451600	1106.34534	1106.350593
7	7	37	8	38	672.603842100	1106.6298	1106.635054
7	10	27	11	27	724.520988300	1106.6299	1106.635154
7	11	27	12	27	827.731021700	1106.6299	1106.635154
7	10	26	11	26	707.993089700	1106.654	1106.659254
7	11	26	12	26	811.209728900	1106.654	1106.659254
7	10	20	11	20	621.669010800	1106.7326	1106.737855
7	11	20	12	20	724.920213800	1106.7326	1106.737855
7	10	17	11	17	586.766459900	1106.7664	1106.771655
7	11	17	12	17	690.031667200	1106.7664	1106.771655
7	10	16	11	16	576.356305000	1106.7746	1106.779855
7	11	16	12	16	679.625692500	1106.7746	1106.779855
7	9	19	10	20	515.928728200	1106.85697	1106.862225
7	8	29	9	30	582.309202600	1106.9455	1106.950756
7	7	38	8	39	695.874332000	1107.3166	1107.321858
7	9	20	10	21	528.179321100	1107.45858	1107.463838
7	8	30	9	31	600.683577900	1107.54575	1107.551009
7	7	39	8	40	719.755696500	1108.0169	1108.022161
7	9	21	10	22	541.042015500	1108.05806	1108.063321
7	8	31	9	32	619.669487700	1108.14539	1108.150651
7	9	22	10	23	554.516748800	1108.65956	1108.664824
7	8	32	9	33	639.266838900	1108.74525	1108.750514
7	9	23	10	24	568.603455300	1109.25899	1109.264257
7	8	33	9	34	659.475535500	1109.34485	1109.350117

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ (K=6) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	9	24	10	25	583.302066500	1109.85767	1109.86294
7	8	34	9	35	680.295478700	1109.94477	1109.95004
7	9	25	10	26	598.612510600	1110.45636	1110.461632
7	8	35	9	36	701.726566300	1110.54344	1110.548713
7	9	26	10	27	614.534713200	1111.05409	1111.059365
7	8	36	9	37	723.768693500	1111.14305	1111.148326
7	9	27	10	28	631.068596500	1111.65181	1111.657088
7	8	37	9	38	746.421752200	1111.74259	1111.747869
7	9	28	10	29	648.214080100	1112.24872	1112.254001
7	8	38	9	39	769.685631500	1112.34278	1112.348061
7	9	29	10	30	665.971080200	1112.84525	1112.850534
7	12	25	13	25	908.257682800	1112.9106	1112.915884
7	12	24	13	24	892.965607700	1112.9251	1112.930384
7	12	22	13	22	864.214852300	1112.9506	1112.955884
7	12	21	13	21	850.756309900	1112.963	1112.968284
7	12	19	13	19	825.673218300	1112.9884	1112.993684
7	12	18	13	18	814.048789400	1112.9987	1113.003985
7	9	30	10	31	684.339510400	1113.44081	1113.446097
7	8	40	9	41	818.045392600	1113.54407	1113.549357
7	9	31	10	32	703.319281100	1114.0361	1114.041389
7	8	41	9	42	843.141037300	1114.14517	1114.15046
7	10	10	11	11	526.751052600	1114.15535	1114.16064
7	11	11	12	12	636.774566600	1114.15535	1114.16064
7	9	32	10	33	722.910299800	1114.63078	1114.636072
7	10	11	11	12	533.487949200	1114.76006	1114.765353
7	11	12	12	13	644.120816100	1114.76006	1114.765353
7	9	33	10	34	743.112470800	1115.22467	1115.229965
7	8	43	9	44	895.163240100	1115.35079	1115.356086
7	10	12	11	13	540.837154400	1115.364	1115.369296
7	11	13	12	14	652.079093300	1115.364	1115.369296
7	9	34	10	35	763.925695700	1115.81855	1115.823848

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^{-1}$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	8	44	9	45	922.089543000	1115.95617	1115.961469
7	10	13	11	14	548.798632600	1115.96719	1115.972489
7	11	14	12	15	660.649359800	1115.96719	1115.972489
7	9	35	10	36	785.349873000	1116.41135	1116.416651
7	8	45	9	46	949.625805200	1116.5629	1116.568201
7	10	14	11	15	557.372345300	1116.57071	1116.576011
7	11	15	12	16	669.831574300	1116.57071	1116.576011
7	9	36	10	37	807.384898000	1117.00407	1117.009374
7	10	15	11	16	566.558251000	1117.17201	1117.177314
7	11	16	12	17	679.625692500	1117.17201	1117.177314
7	9	37	10	38	830.030663300	1117.5962	1117.601506
7	10	16	11	17	576.356305000	1117.77299	1117.778297
7	11	17	12	18	690.031667200	1117.77299	1117.778297
7	9	38	10	39	853.287058400	1118.18815	1118.193459
7	10	17	11	18	586.766459900	1118.37349	1118.3788
7	11	18	12	19	701.049448200	1118.37349	1118.3788
7	9	39	10	40	877.153969800	1118.77878	1118.784092
7	10	18	11	19	597.788665300	1118.97394	1118.979253
7	11	19	12	20	712.678982400	1118.97394	1118.979253
7	9	40	10	41	901.631280800	1119.36954	1119.374855
7	10	19	11	20	609.422867800	1119.57367	1119.578986
7	11	20	12	21	724.920213800	1119.57367	1119.578986
7	9	41	10	42	926.718872200	1119.96005	1119.965368
7	10	20	11	21	621.669010800	1120.17218	1120.177499
7	11	21	12	22	737.773083300	1120.17218	1120.177499
7	9	42	10	43	952.416621300	1120.54962	1120.55494
7	12	12	13	13	757.145178700	1120.99837	1121.003693
7	9	43	10	44	978.724402600	1121.1397	1121.145023
7	10	22	11	23	647.996878400	1121.36884	1121.374164
7	11	23	12	24	765.313485600	1121.36884	1121.374164
7	12	13	13	14	765.099955100	1121.60184	1121.607165

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ (K=6) bands of CH₃CN.

Band	k''	j''	k'	j'	Ground.State Energy (cm ⁻¹)	Transition Energy (cm ⁻¹)	Calibrated Transition Energy (cm ⁻¹)
7	9	44	10	45	1005.642088000	1121.72878	1121.734106
7	10	23	11	24	662.078475200	1121.96608	1121.971407
7	11	24	12	25	780.000885600	1121.96608	1121.971407
7	12	14	13	15	773.666452600	1122.20474	1122.210068
7	9	45	10	46	1033.169545000	1122.31762	1122.322949
7	10	24	11	25	676.771757400	1122.56264	1122.56797
7	11	25	12	26	795.299657900	1122.56264	1122.56797
7	12	15	13	16	782.844630300	1122.80754	1122.812871
7	9	46	10	47	1061.306640000	1122.90602	1122.911352
7	10	25	11	26	692.076653600	1123.15167	1123.157003
7	11	26	12	27	811.209728900	1123.15167	1123.157003
7	12	16	13	17	792.634444100	1123.40905	1123.414384
7	9	47	10	48	1090.053235000	1123.49365	1123.498984
7	12	17	13	18	803.035847100	1124.01035	1124.015687
7	9	48	10	49	1119.409190000	1124.08184	1124.087177
7	12	18	13	19	814.048789400	1124.61182	1124.61716
7	9	49	10	50	1149.374361000	1124.66939	1124.67473
7	10	28	11	29	741.660269400	1124.93752	1124.942861
7	11	29	12	30	862.606950700	1124.93752	1124.942861
7	12	19	13	20	825.673218300	1125.21148	1125.216823
7	9	50	10	51	1179.948601000	1125.25612	1125.261463
7	10	29	11	30	759.410849800	1125.53097	1125.536314
7	11	30	12	31	880.961418600	1125.53097	1125.536314
7	12	20	13	21	837.909078000	1125.81093	1125.816275
7	9	51	10	52	1211.131762000	1125.84425	1125.849596
7	12	21	13	22	850.756309900	1126.40965	1126.414998
7	9	52	10	53	1242.923690000	1126.43178	1126.437128
7	12	22	13	23	864.214852300	1127.00852	1127.013871
7	10	32	11	33	816.329510400	1127.34791	1127.353263
7	11	33	12	34	939.689763600	1127.34791	1127.353263
7	12	23	13	24	878.284640800	1127.60575	1127.611104

Table A.1 (cont.)

Transition assignments for the ν_7 and $3\nu_8^1$ ($K=6$) bands of CH_3CN .

Band	k''	j''	k'	j'	Ground.State Energy (cm^{-1})	Transition Energy (cm^{-1})	Calibrated Transition Energy (cm^{-1})
7	10	33	11	34	836.524396700	1127.95085	1127.956206
7	11	34	12	35	960.487210600	1127.95085	1127.956206
7	12	24	13	25	892.965607700	1128.20315	1128.208507
7	10	34	11	35	857.330121900	1128.55338	1128.558738
7	11	35	12	36	981.895158500	1128.55338	1128.558738

Appendix B

Program listing for controlling the grating stepper motor of the tunable diode laser (TDL) spectrometer. In addition, the program also controls the stepper motor for a sun tracker being developed by Stewart Hager of UTMSL. The program was written in Visual Basic for Windows and was developed by Alan Ewing of UTMSL and by the author. There are a total of 5 program listings for the controller program given in this appendix. These files have extensions of BAS for BASIC code only and FRM for form code which generates the graphical user interface (GUI) and also contains BASIC subroutines.

SC149A2.BAS

'TDL and Heliostat Control Program
'University of Tennessee Molecular Spectroscopy Lab
'written by Alan Ewing and Larry Jennings
'some routines from public domain

'Following function and sub needed to communicate with the
'Alpha Products card. Works the same as the Quick Basic
'INP and OUT functions.

Declare Function Inp Lib "inout.dll" (ByVal Port%) As Integer
Declare Sub out Lib "inout.dll" (ByVal Port%, ByVal Value%)

Dim s2(35), f2(35), y2(35), u(100), X(35), Y(35) As Double

'Reply is the string containing the reply from the SC-149

Global reply

'Setup the required variables and strings for communication
'with the signal averager. Some not used in this program yet.
'From COMMDEMO public domain listing
'Communications etc. declarations and global variables
Type CommStateDCB

 Id As String * 1 ' Port Id from OpenComm
 BaudRate As Integer ' Baud Rate
 ByteSize As String * 1 ' Data Bit Size (4 to 8)
 Parity As String * 1 ' Parity
 StopBits As String * 1 ' Stop Bits
 RlsTimeout As Integer ' Carrier Detect Time "CD"

```

CtsTimeOut As Integer ' Clear-to-Send Time
DsrTimeOut As Integer ' Data-Set-Ready Time
ModeControl As Integer ' Mode Control Bit Fields
XonChar As String * 1 ' XON character
XoffChar As String * 1 ' XOFF character
XonLim As Integer ' Min characters in buffer before XON is sent
XoffLim As Integer ' Max characters in buffer before XOFF is send
PeChar As String * 1 ' Parity Error Character
EofChar As String * 1 ' EOF/EOD character
EvtChar As String * 1 ' Event character
TxDelay As Integer ' Reserved/Not Used
End Type

```

```

Type TextMetrics
    tmHeight As Integer
    work1 As String * 14
    work2 As String * 9
    Work3 As String * 6
End Type

```

```

Declare Function OpenComm Lib "user" (ByVal a As String) : ', ByVal b As Integer, ByVal c As Integer)
As Integer
Declare Function CloseComm Lib "user" (ByVal a As Integer) As Integer

```

```

Declare Function WriteComm Lib "user" (ByVal a As Integer, ByVal b As String, ByVal c As Integer) As
Integer
Declare Function ReadComm Lib "user" (ByVal a As Integer, ByVal b As String, ByVal c As Integer) As
Integer

```

```

Declare Function GetCommEventMask Lib "user" (ByVal a As Integer, ByVal b As Integer) As Integer
Declare Function SetCommEventMask Lib "user" (ByVal a As Integer, ByVal b As Integer) As Integer

```

```

Declare Function SetCommState Lib "user" (b As CommStateDCB) As Integer
Declare Function GetCommState Lib "user" (ByVal a As Integer, b As CommStateDCB) As Integer

```

```

Declare Function RemoveMenu Lib "User" (ByVal hMenu As Integer, ByVal nPosition As Integer, ByVal
wFlags As Integer) As Integer
Declare Function GetSystemMenu Lib "User" (ByVal hWnd As Integer, ByVal Action As Integer) As
Integer
Global Const false1 = 0
Global Const true1 = Not false1

```

```

Global Const MF_BYPOSITION = &H400 'Used by RemoveMenu()

```

```

' COMM OPEN Error Numbers

```

```

Global Const IE_BADID = -1 ' Invalid or unsupported id
Global Const IE_OPEN = -2 ' Device Already Open
Global Const IE_NOPEN = -3 ' Device Not Open
Global Const IE_MEMORY = -4 ' Unable to allocate queues
Global Const IE_DEFAULT = -5 ' Error in default parameters

```

Global Const IE_HARDWARE = -10 ' Hardware Not Present
Global Const IE_BYTESIZE = -11 ' Illegal Byte Size
Global Const IE_BAUDRATE = -12 ' Unsupported BaudRate

' COMM EVENT MASK

Global Const EV_RXCHAR = &H1
Global Const EV_RXFLAG = &H2
Global Const EV_TXEMPTY = &H4
Global Const EV_CTS = &H8
Global Const EV_DSR = &H10
Global Const EV_RLSD = &H20
Global Const EV_BREAK = &H40
Global Const EV_ERR = &H80
Global Const EV_RING = &H100
Global Const EV_PERR = &H200
Global Const EV_ALL = &H3FF

Global CommHandle As Integer
Global CommDeviceNum As Integer

Global CommPortName As String
Global PostPortName As String

Global CommEventMask As Integer
Global PostEventMask As Integer

Global CommState As CommStateDCB
Global PostState As CommStateDCB

Global CommRBBuffer As Integer
Global PostRBBuffer As Integer

Global CommTBBuffer As Integer
Global PostTBBuffer As Integer

Global CommReadInterval As Integer
Global PostReadInterval As Integer

Global CaptionLeft As Integer
Global CaptionTop As Integer
Global CaptionHeight As Integer
Global CaptionCenter As Integer
Global CaptionWidth As Integer
Global CaptionText\$

' Some more variables that are to be used for comm port

Global larry\$(2048): 'holds the values read from comm port
Global flag, dump
Global counter: 'keeps track of the number of items read from comm port

Global b1\$

Sub getcalfile (s2(), f2(), numinfi)

'The calibration file must be read in to insure the conversion
'from stepper motor position to wavenumber.

Debug.Print numinfi;

Open "c:\diode\cal2.dta" For Input As #1

Input #1, numinfi

For conter = 1 To numinfi

Input #1, s2(conter), f2(conter)

Next conter

235 Close #1

End Sub

Sub listening (flagal, reply)

'Debug.Print "called by: "; flagal

For mqe = 1 To 3000: Next mqe

reply = ""

937 If (Inp(522 + 1) And 64) = 0 Then

reply = reply + Chr\$(Inp(522))

Else

GoTo 938

End If

For mqe = 1 To 50: Next mqe

GoTo 937

938 If Right\$(reply, 1) = Chr\$(13) Then

reply = Left\$(reply, Len(reply) - 1)

If flagal = 0 Then motorcntrl!receive.Text = reply

If flagal = 1 Then

motorcntrl!heliostepnotext.Text = reply

helio!heliopos.Text = reply

End If

If flagal = 2 Then

motorcntrl!tdlstepnotext.Text = reply

tdlfrm!tdlposbox.Text = reply

End If

If flagal = 3 Then helio!heliospdbox.Text = reply

If flagal = 4 Then tdlfrm!tdlcurrentspeedtext.Text = reply

End If

939 End Sub

Sub Main ()

motorcntrl.Show 'Optionally, you can load and display a form.

Rem For dlay = 1 To 10: Next dlay

Call getcalfile(s2(), f2(), a)

Call SPLINE(s2(), f2(), a, 1E+30, 1E+30, y2())

Do While DoEvents()

ww = ww + 1

If ww = 500 Then

```

    outptr$ = "pos1"
    ' Debug.Print "from1"
    Call talking(outptr$)
    For mq = 1 To 1000: Next mq
    Call listening(1, resp)
End If

If ww = 1000 Then
    outptr$ = "sp1"
    Call talking(outptr$)
    For mq = 1 To 1000: Next mq
    ' Debug.Print "from3"
    Call listening(3, resp)
End If
If ww = 1500 Then
    outptr$ = "pos2"
    Call talking(outptr$)
    For mq = 1 To 1000: Next mq
    ' Debug.Print "from2"
    Call listening(2, resp)
    resp1 = Val(resp)
    ' Debug.Print resp1, resp
    Call SPLINT(s2(), f2(), y2(), a, resp1, resp2)
    resp3 = Str$(resp2)
    motorcntrl!tdlfreqnotext.Text = resp3
    tdlfrm!tdlkaiserbox.Text = resp3
End If
If ww = 2000 Then
    outptr$ = "sp2"
    Call talking(outptr$)
    For mq = 1 To 1000: Next mq
    Call listening(4, resp)
ww = 0
End If
'Place idle-loop code here. These statements are processed
'whenever the system has free time

'Debug.Print "i'm in the idle loop " + r
'r = r + 1
' if r > 32000 Then r = 0
'let's listen to the sc149 since we are not doing anything
' Call listening(0)
Rem Call heliogetpos
Loop
End Sub

Sub SPLINE (X(), Y(), N, YP1, YPN, d2())

    'Debug.Print "I'm here"
    If YP1 > 9.9E+29 Then
        d2(1) = 0#
    
```

```

    u(1) = 0#
Else
    d2(1) = -.5
    u(1) = (3# / (X(2) - X(1))) * ((Y(2) - Y(1)) / (X(2) - X(1)) - YP1)
End If
For i = 2 To N - 1
    SIG = (X(i) - X(i - 1)) / (X(i + 1) - X(i - 1))
    P = SIG * d2(i - 1) + 2#
    d2(i) = (SIG - 1#) / P
    'Debug.Print n, i, y(i + 1), y(i), x(i + 1), x(i)
    u(i) = (Y(i + 1) - Y(i)) / (X(i + 1) - X(i))
    u(i) = (u(i) - (Y(i) - Y(i - 1)) / (X(i) - X(i - 1))) / (X(i + 1) - X(i - 1))
    u(i) = 6# * (u(i) - SIG * u(i)) / P
'    U(I)=(6.E0*((Y(I+1)-Y(I))/(X(I+1)-X(I))-(Y(I)-Y(I-1))
'    *    /(X(I)-X(I-1)))/(X(I+1)-X(I-1))-SIG*U(I-1))/P

Next i
If YPN > 9.9E+29 Then
    QN = 0#
    UN = 0#
Else
    QN = .5
    UN = (3# / (X(N) - X(N - 1))) * (YPN - (Y(N) - Y(N - 1)) / (X(N) - X(N - 1)))
End If
d2(N) = (UN - QN * u(N - 1)) / (QN * d2(N - 1) + 1#)
For K = N - 1 To 1 Step -1
    d2(K) = d2(K) * d2(K + 1) + u(K)
Next K
End Sub

Sub SPLINT (XA(), YA(), Y2A(), N, X, Y)
    KLO = 1
    KHI = N
50200 If KHI - KLO > 1 Then
    K = (KHI + KLO) / 2
    If XA(K) > X Then
        KHI = K
    Else
        KLO = K
    End If
    GoTo 50200
End If
H = XA(KHI) - XA(KLO)
If H = 0# Then Exit Sub

a = (XA(KHI) - X) / H
b = (X - XA(KLO)) / H
Y = a * YA(KLO) + b * YA(KHI)
Y = Y + ((a ^ 3 - a) * Y2A(KLO) + (b ^ 3 - b) * Y2A(KHI)) * (H ^ 2) / 6#
End Sub

```

```

Sub talking (motorcmd)
'Debug.Print "command received: "; motorcmd
If motorcmd = "" Then 32001
For mqe = 1 To 5000: Next mqe
motorcmd = motorcmd + Chr$(13)
For yyy = 1 To Len(motorcmd)
    For w = 1 To 3500: Next w: Rem Delay here
xxx = Asc(Mid$(motorcmd, yyy, 1))
'Debug.Print x, Chr$(x)
551 out 522, xxx: Next yyy: GoTo 32001
32001 Rem ***** time to quit talking to sc149*****
End Sub

```

```

Sub talktosigave (comd1$)
send$ = comd1$
    WriteCommPort comd1$ + Chr$(13)
End Sub

```

SC149A2.FRM

VERSION 2.00

Begin Form motorcntrl

Caption = "Motor Control"

Height = 4950

Left = 1110

LinkTopic = "Form1"

ScaleHeight = 4260

ScaleWidth = 7365

Top = 1440

Width = 7485

Begin TextBox tdlfreqnotext

Height = 495

Left = 6000

TabIndex = 14

Top = 1800

Width = 1215

End

Begin TextBox tdlstepnotext

Height = 495

Left = 4560

TabIndex = 13

Top = 1800

Width = 1215

End

Begin TextBox heliostepnotext

Height = 495

Left = 4560

TabIndex = 12

```

    Top      = 720
    Width    = 1215
End
Begin CommandButton quitbutton
    Caption   = "Quit"
    Height    = 495
    Left      = 5520
    TabIndex  = 5
    Top       = 3240
    Width     = 1695
End
Begin TextBox receive
    Height    = 375
    Left      = 120
    TabIndex  = 3
    Top       = 3240
    Width     = 1575
End
Begin CommandButton sendbutton
    Caption   = "Ok"
    Height    = 375
    Left      = 480
    TabIndex  = 2
    Top       = 1920
    Width     = 855
End
Begin TextBox send
    Height    = 375
    Left      = 240
    TabIndex  = 0
    Top       = 1440
    Width     = 1335
End
Begin Label tdlfreqlabel
    Alignment = 2 'Center
    Caption   = "Frequency"
    Height    = 255
    Left      = 6000
    TabIndex  = 11
    Top       = 1440
    Width     = 1215
End
Begin Label tdlstepnolabel
    Alignment = 2 'Center
    Caption   = "Step Number"
    Height    = 255
    Left      = 4560
    TabIndex  = 10
    Top       = 1440
    Width     = 1215
End

```

```

Begin Label heliostepnolabel
  Alignment    = 2 'Center
  Caption      = "Step Number"
  Height       = 255
  Left         = 4560
  TabIndex     = 9
  Top          = 240
  Width        = 1215
End
Begin Label tdlgratposlabel
  Alignment    = 2 'Center
  Caption      = "TDL Grating Position"
  Height       = 495
  Left         = 3120
  TabIndex     = 8
  Top          = 1800
  Width        = 1215
End
Begin Label helioposlabel
  Alignment    = 2 'Center
  Caption      = "Heliostat Position"
  Height       = 375
  Left         = 3120
  TabIndex     = 7
  Top          = 720
  Width        = 1215
End
Begin Label dircntrllabel
  Alignment    = 2 'Center
  Caption      = "Direct Contol"
  Height       = 375
  Left         = 240
  TabIndex     = 6
  Top          = 240
  Width        = 1455
End
Begin Label sc149replytext
  Alignment    = 2 'Center
  Caption      = "Last Reply From SC-149"
  Height       = 375
  Left         = 120
  TabIndex     = 4
  Top          = 2760
  Width        = 1575
End
Begin Label cmd2sc149label
  Caption      = " Command to      SC-149"
  Height       = 375
  Left         = 240
  TabIndex     = 1
  Top          = 960

```

```

    Width      = 1335
End
Begin Menu TDL
    Caption    = "&TDL"
    Index      = 1
End
Begin Menu Heliostat
    Caption    = "&Heliostat"
    Index      = 1
End
Begin Menu about1
    Caption    = "&About"
    Index      = 1
End
End
Declare Function Inp Lib "inpout.dll" (ByVal Port%) As Integer
Declare Sub out Lib "inpout.dll" (ByVal Port%, ByVal Value%)

Dim motorcmd
Dim reply

Sub ABOUT_Click (Index As Integer)
about.Show 0
Rem

End Sub

Sub about1_Click (Index As Integer)
about.Show
End Sub

Sub Form_Load ()
    Call Initialize

    'Menu_Comm_Connect.Visible = true
    'Menu_Comm_Disconnect.Visible = false

    'offset = 200

    'CaptionLeft = offset
    'CaptionTop = offset
    'CaptionWidth = ScaleWidth - CaptionLeft - offset
    'CaptionHeight = TextHeight("qypgjXAQK") * 1.5

    'UpdateCaption " Ready", 0

    'Left = (Screen.Width - Width) / 2
    'top = Height - ScaleHeight
    'Height = top + CaptionTop + CaptionHeight + offset

```

End Sub

Sub Heliostat_Click (Index As Integer)

helio.Show

Rem

End Sub

Sub Initialize ()

IndexTrans = 0

IndexReceive = 0

CommHandle = -1

CommDeviceNum = -1

' Default Port Settings

CommPortName = "COM1:"

CommState.BaudRate = 1200

CommState.ByteSize = Chr\$(7)

CommState.Parity = Chr\$(2)

CommState.StopBits = Chr\$(2)

' Default Line Settings

CommRBBuffer = 2048

CommTBBuffer = 2048

CommState.RtsTimeOut = 0

CommState.CtsTimeOut = 0

CommState.DsrTimeOut = 0

CommEventMask = &H3FF

CommReadInterval = 500

' Post-Poned settings

PostRBBuffer = CommRBBuffer

PostTBBuffer = CommTBBuffer

PostEventMask = CommEventMask

PostState = CommState

PostReadInterval = CommReadInterval

PostPortName = CommPortName

End Sub

Sub quitbutton_Click ()

End

End Sub

Sub receive_change ()

```
Rem receive.Text = motorcmd
```

```
End Sub
```

```
Sub sendbutton_Click ()
```

```
outprt2$ = send.Text  
'Debug.Print send.Text  
Call talking(outprt2$)
```

```
Call listening(0, resp)
```

```
End Sub
```

```
Sub TDL_Click (Index As Integer)
```

```
tdlfrm.Show 0
```

```
Rem
```

```
End Sub
```

TDL2.FRM

VERSION 2.00

Begin Form tdlfrm

Caption = "TDL"

Height = 6630

Left = 1050

LinkTopic = "Form3"

ScaleHeight = 5940

ScaleWidth = 7950

Top = 1275

Width = 8070

Begin TextBox datanametext

Height = 375

Left = 4320

TabIndex = 31

Text = "default.dta"

Top = 480

Width = 1935

End

Begin Timer sigavereceive_timer

Left = 7320

Top = 4080

End

Begin Frame tdlmotorcntrlframe

Caption = "TDL Motor Control"

Height = 5415

Left = 120

TabIndex = 4

```

Top      = 120
Width    = 3255
Begin CommandButton tdlmovetobutton
Caption  = "Move To"
Height   = 375
Left     = 960
TabIndex = 27
Top      = 1440
Width    = 1215
End
Begin Frame tdlmotioncntrlframe
Caption  = "Motion Control"
Height   = 1575
Left     = 120
TabIndex = 16
Top      = 1920
Width    = 3015
Begin Frame tdlDIRcntrlframe
Caption  = "Direction"
Height   = 855
Left     = 120
TabIndex = 26
Top      = 600
Width    = 2775
Begin OptionButton tdlnegdiroption
Caption  = "Negative"
Height   = 375
Left     = 1440
TabIndex = 29
Top      = 360
Width    = 1335
End
Begin OptionButton tdlposdiroption
Caption  = "Positive"
Height   = 375
Left     = 120
TabIndex = 28
Top      = 360
Value    = -1 'True
Width    = 1215
End
End
Begin OptionButton tdlrestoption
Caption  = "Rest"
Height   = 375
Left     = 2040
TabIndex = 19
Top      = 240
Value    = -1 'True
Width    = 855
End

```

```

Begin OptionButton tdlstopoption
  Caption      = "Stop"
  Height       = 375
  Left         = 960
  TabIndex     = 18
  Top          = 240
  Width        = 855
End
Begin OptionButton tdlgooption
  Caption      = "Go"
  Height       = 375
  Left         = 120
  TabIndex     = 17
  Top          = 240
  Width        = 735
End
Begin Frame tdlmotorspeedframe
  Caption      = "Motor Speed"
  Height       = 1815
  Left         = 120
  TabIndex     = 9
  Top          = 3480
  Width        = 3015
Begin TextBox tdlcurrentspeedtext
  Height       = 360
  Left         = 1080
  TabIndex     = 15
  Top          = 1440
  Width        = 855
End
Begin CommandButton tdl speedsendbutton
  Caption      = "Send"
  Height       = 255
  Left         = 1560
  TabIndex     = 13
  Top          = 720
  Width        = 1095
End
Begin TextBox tdl speedtext
  Height       = 360
  Left         = 480
  TabIndex     = 12
  Top          = 720
  Width        = 615
End
Begin HScrollBar tdl speedscrollbar
  Height       = 240
  Left         = 120
  Max          = 100
  Min          = 1

```

```

    TabIndex    = 11
    Top         = 360
    Value       = 25
    Width       = 2655
End
Begin Label tdlcurrentspeedlabel
    Alignment    = 2 'Center
    Caption      = "Current Speed"
    Height       = 255
    Left         = 720
    TabIndex     = 14
    Top          = 1200
    Width        = 1455
End
End
Begin TextBox tdlkaiserbox
    Height       = 495
    Left         = 1680
    TabIndex     = 6
    Top          = 840
    Width        = 1335
End
Begin TextBox tdlposbox
    Height       = 495
    Left         = 120
    TabIndex     = 5
    Top          = 840
    Width        = 1335
End
Begin Label tdlgratposlabel
    Alignment    = 2 'Center
    Caption      = "TDL Grating Position"
    Height       = 255
    Left         = 600
    TabIndex     = 10
    Top          = 360
    Width        = 1935
End
Begin Label tdlkaisernolabel
    Alignment    = 2 'Center
    Caption      = "Wavenumbers"
    Height       = 255
    Left         = 1560
    TabIndex     = 8
    Top          = 600
    Width        = 1575
End
Begin Label tdlstepnolabel
    Alignment    = 2 'Center
    Caption      = "Step Numbers"
    Height       = 255

```

```

    Left      = 120
    TabIndex  = 7
    Top       = 600
    Width     = 1335
End
End
Begin Frame sigavgcntrlframe
    Caption   = "Signal Averager Control"
    Height    = 2775
    Left      = 3600
    TabIndex  = 1
    Top       = 960
    Width     = 3975
Begin CommandButton viewdatbutton
    Caption   = "View Data"
    Height    = 375
    Left      = 2280
    TabIndex  = 25
    Top       = 960
    Width     = 1575
End
Begin Frame sigavgscanframe
    Caption   = "Scan Control"
    Height    = 1935
    Left      = 120
    TabIndex  = 20
    Top       = 360
    Width     = 2055
Begin OptionButton stopoption
    Caption   = "Stop"
    Height    = 375
    Left      = 120
    TabIndex  = 24
    Top       = 1440
    Width     = 1215
End
Begin OptionButton startoption
    Caption   = "Start"
    Height    = 375
    Left      = 120
    TabIndex  = 23
    Top       = 1080
    Width     = 1095
End
Begin OptionButton clrswEEPoption
    Caption   = "Clear Sweeps"
    Height    = 375
    Left      = 120
    TabIndex  = 22
    Top       = 720
    Width     = 1815

```

```

End
Begin OptionButton clrmemoryoption
  Caption      = "Clear Memory"
  Height       = 375
  Left         = 120
  TabIndex     = 21
  Top          = 360
  Width        = 1815
End
End
Begin CommandButton abortscanbutton
  Caption      = "ABORT SCAN!"
  Height       = 855
  Left         = 2280
  TabIndex     = 3
  Top          = 1440
  Width        = 1575
End
Begin CommandButton retrievedatbutton
  Caption      = "Retrieve Data"
  Height       = 375
  Left         = 2280
  TabIndex     = 2
  Top          = 480
  Width        = 1575
End
End
Begin CommandButton tdlexitbutton
  Caption      = "Exit"
  FontBold     = -1 'True
  FontItalic   = 0 'False
  FontName     = "MS Sans Serif"
  FontSize     = 24
  FontStrikethru = 0 'False
  FontUnderline = 0 'False
  Height       = 855
  Left         = 5520
  TabIndex     = 0
  Top          = 4560
  Width        = 1815
End
Begin Label datnamelabel
  Caption      = "Data Filename"
  Height       = 255
  Left         = 4320
  TabIndex     = 30
  Top          = 120
  Width        = 1815
End
Begin Menu Fileaces
  Caption      = "&File"

```

```

Begin Menu savfile
    Caption    = "&Save"
End
Begin Menu delfile
    Caption    = "&Delete"
End
End
Begin Menu caltdl
    Caption    = "&Calibrate"
End
Begin Menu tdlcomm
    Caption    = "C&ommunications"
    Begin Menu tdl_menu_com_connect
        Caption    = "Connect"
        Shortcut    = ^C
    End
    Begin Menu tdl_menu_comm_disconnect
        Caption    = "Disconnect"
        Shortcut    = ^D
    End
End
End
Dim larry$(2049)

Dim dump

Sub abortscanbutton_Click ()

comd1$ = "TE"
Call talktosigave(comd1$)

End Sub

Sub Clearmem_Click ()

End Sub

Sub clearreceive ()
'For x = 1 To 2
a$ = ReadCommPort(128)
'Next x
End Sub

Sub clrmemoption_Click ()

    dump = 0
    comd1$ = "CM"
    Call talktosigave(comd1$)
    dump = 1
    Call sigavereceive_timer_Timer

```

End Sub

```
Sub clrswEEPoption_Click ()  
dump = 0  
comd1$ = "CS"  
Call talktosigave(comd1$)  
dump = 1  
Call sigavereceive_timer_Timer
```

End Sub

```
Sub dumpdata ()  
1 counter = counter + 1  
a$ = ReadCommPort(128)  
larry$(counter) = a$  
b1$ = a$  
If counter < 2048 Then 1
```

End Sub

```
Sub retrievedatbutton_Click ()  
dump = 2  
comd1$ = "DP,0000,2047,A"  
Call talktosigave(comd1$)  
Call sigavereceive_timer_Timer
```

```
Call tofile  
'dump = 3  
'comd1$ = "SE-AL"  
'Call talktosigave(comd1$)  
'Call sigavereceive_timer
```

End Sub

```
Sub savfile_Click ()  
Call tofile  
End Sub
```

```
Sub sigavereceive_timer_Timer ()  
  
If dump = 1 Then Call clearreceive  
If dump = 2 Then Call dumpdata
```

dump = 0

End Sub

```
Sub sigavereceive_timer1 ()  
If dump = 1 Then Call clearreceive  
If dump = 2 Then Call dumpdata
```

```
'If flag = 1 Then tofile
```

```
'If Len(a$) > 0 Then
```

```
    'Receive_Text.SelStart = Len(Receive_Text.Text) + 1
```

```
    'Receive_Text.SelLength = 0
```

```
    'Receive_Text.SelText = a$
```

```
'larry$(counter) = a$
```

```
'End If
```

```
End Sub
```

```
Sub startoption_Click ()
```

```
    dump = 0
```

```
    comd1$ = "GO"
```

```
    Call talktosigave(comd1$)
```

```
    dump = 1
```

```
    Call sigavereceive_timer_Timer
```

```
End Sub
```

```
Sub stopoption_Click ()
```

```
    dump = 0
```

```
    comd1$ = "HT"
```

```
    Call talktosigave(comd1$)
```

```
    dump = 1
```

```
    Call sigavereceive_timer_Timer
```

```
End Sub
```

```
Sub tdl_menu_com_connect_Click ()
```

```
    'UpdateCaption " Opening Comm Port..." + CommPortName, .5
```

```
    CommTBBuffer = PostTBBuffer
```

```
    CommRBBuffer = PostRBBuffer
```

```
    CommPortName = PostPortName
```

```
    CommHandle = OpenComm(CommPortName): ', CommRBBuffer, CommTBBuffer)
```

```
    If CommHandle = -2 Then
```

```
        result% = MsgBox("Port already Open!" + Chr$(13) + "Do you want to use it anyway ?", 4 + 16 +  
256, "Communication Sampler II")
```

```
        If result% = 6 Then
```

```
            ApiErr% = CloseComm(0)
```

```
            CommHandle = OpenComm(CommPortName): ', CommRBBuffer, CommTBBuffer)
```

```
        End If
```

```
    End If
```

```

If CommHandle < 0 Then
    'UpdateCaption " OpenComm() API Failed! (ERR " + Str$(CommHandle) + ")", .5
Else
    'Menu_Windows.Enabled = true1
    'Menu_Window_Receive_Transmit.Checked = true1

    'Receive.Show

    CommEventMask = PostEventMask
    CommDeviceNum = Val(Mid$(CommPortName, 4, 1))
    ApiErr% = SetCommEventMask(CommHandle, CommEventMask)

    PostState = CommState
    CommState.Id = Chr$(CommHandle)

    ApiErr% = SetCommState(CommState)

    'Menu_Comm_Connect.Visible = Menu_Comm_Disconnect.Visible
    'Menu_Comm_Disconnect.Visible = Not Menu_Comm_Connect.Visible
    'UpdateCaption " Commuications Port Opened...", .5
    DisplayQBOpen CommState, CommPortName, CommRBBuffer, CommTBBuffer,
CommReadInterval

    CommReadInterval = PostReadInterval
    tdlfrm!sigavereceive_timer.Interval = CommReadInterval
End If

End Sub

Sub tdl_menu_comm_disconnect_Click ()

    'UpdateCaption " Closing Communication Port...", 0

    tdlfrm!sigavereceive_timer.Interval = 0

    ApiErr% = CloseComm(CommHandle)
    CommHandle = -1
    CommDeviceNum = -1

    'Menu_Comm_Disconnect.Visible = Menu_Comm_Connect.Visible
    'Menu_Comm_Connect.Visible = Not Menu_Comm_Disconnect.Visible

    'Menu_Windows.Enabled = false1
    'Unload Receive

    'UpdateCaption " Ready", 0

End Sub

```

```
Sub tdlexitbutton_Click ()
tdlfrm.Hide
End Sub
```

```
Sub tdlgooption_Click ()
If tdlposdiroption = True Then sufx$ = " pd"
If tdlnegdiroption = True Then sufx$ = " nd"
comd$ = "go2" + sufx$
Call talking(comd$)

End Sub
```

```
Sub tdlrestoption_Click ()

comd$ = "rest2"
Call talking(comd$)

End Sub
```

```
Sub tdlspeedscrollbar_Change ()

tdlspeedtext.Text = tdlspeedscrollbar.Value

End Sub
```

```
Sub tdlspeedsendbutton_Click ()

comd$ = "sp2 " + tdlstext.Text
Call talking(comd$)

End Sub
```

```
Sub tdlstopoption_Click ()

comd$ = "stop2"
Call talking(comd$)

End Sub
```

```
Sub tofile ()
datafile$ = tdlfrm!datnametext.Text

Open datafile$ For Output Access Write As #1

For X = 1 To 2048
Print #1, , larry$(X)
Next X
Close #1

End Sub
```

HELIO2.FRM

VERSION 2.00

Begin Form Helio

Caption = "Heliostat"
Height = 4545
Left = 2145
LinkTopic = "Form2"
ScaleHeight = 4020
ScaleWidth = 7365
Top = 1905
Width = 7485

Begin Frame speedcntrlframe

Caption = "Speed Control"
Height = 1455
Left = 240
TabIndex = 9
Top = 2400
Width = 3015

Begin HScrollBar speedcntrlbar

Height = 255
Left = 120
Max = 200
Min = 1
TabIndex = 15
Top = 480
Value = 1
Width = 2775

End

Begin TextBox sendhelio

Height = 375
Left = 120
TabIndex = 11
Top = 960
Width = 1215

End

Begin CommandButton speedchnngbutton

Caption = "Send Change"
Height = 375
Left = 1560
TabIndex = 10
Top = 960
Width = 1335

End

End

Begin TextBox heliospdbox

Alignment = 2 'Center
Height = 495

```

Left      = 5880
TabIndex  = 8
Top       = 840
Width     = 1215
End
Begin Frame motioncntrlframe
Caption   = "Motion Control"
Height    = 1935
Left      = 240
TabIndex  = 3
Top       = 120
Width     = 3495
Begin Frame dircntrlframe
Caption   = "Direction"
Height    = 1455
Left      = 1800
TabIndex  = 12
Top       = 240
Width     = 1575
Begin OptionButton negdiroption
Caption   = "Negative"
Height    = 375
Left      = 240
TabIndex  = 14
Top       = 960
Width     = 1095
End
Begin OptionButton posdiroption
Caption   = "Positive"
Height    = 375
Left      = 240
TabIndex  = 13
Top       = 480
Value     = -1 'True
Width     = 975
End
End
Begin OptionButton restcntrloption
Caption   = "Rest"
Height    = 375
Left      = 480
TabIndex  = 6
Top       = 1440
Value     = -1 'True
Width     = 1095
End
Begin OptionButton stopcntrloption
Caption   = "Stop"
Height    = 375
Left      = 480
TabIndex  = 5

```

```

    Top      = 960
    Width    = 1095
End
Begin OptionButton gocntrloption
    Caption   = "Go"
    Height    = 375
    Left      = 480
    TabIndex  = 4
    Top       = 480
    Width     = 1095
End
End
Begin CommandButton helioexitbutton
    Caption   = "EXIT"
    FontBold  = -1 'True
    FontItalic = 0 'False
    FontName  = "MS Sans Serif"
    FontSize  = 24
    FontStrikethru = 0 'False
    FontUnderline = 0 'False
    Height    = 975
    Left      = 5400
    TabIndex  = 2
    Top       = 2880
    Width     = 1815
End
Begin TextBox heliopos
    Alignment  = 2 'Center
    Height     = 495
    Left       = 3960
    TabIndex   = 0
    Top        = 840
    Width      = 1455
End
Begin Label heliospeedlabel
    Alignment  = 2 'Center
    Caption    = "Heliostat Motor Speed"
    Height     = 495
    Left       = 5880
    TabIndex   = 7
    Top        = 240
    Width      = 1215
End
Begin Label helioposlabel
    Alignment  = 2 'Center
    Caption    = "Heliostat Motor Position"
    Height     = 495
    Left       = 3960
    TabIndex   = 1
    Top        = 240
    Width      = 1455

```

```

End
End
Dim heliocmd
Dim helioreply

Sub gocntrloption_Click ()
If posdiroption = True Then sufx$ = " pd"
If negdiroption = True Then sufx$ = " nd"
comd$ = "go1" + sufx$
Call talking(comd$)

End Sub

Sub helioexitbutton_Click ()

helio.Hide

End Sub

Sub Restbutton_Click ()
comd$ = "rest1"
Rem
Call talking(comd$)
End Sub

Sub restcntrloption_Click ()
comd$ = "rest1"
Call talking(comd$)

End Sub

Sub sendhelio_Change ()
If (sendhelio.Text > 0 And sendhelio.Text <= 201) Then
    speedcntrlbar.Value = sendhelio.Text
End If
End Sub

Sub speedchnghbutton_Click ()

outprth$ = sendhelio.Text
outprth$ = "sp1 " + outprth$

Call talking(outprth$)

Call listening(3, resp)

End Sub

Sub speedcntrlbar_Change ()

```

```
sendhelio.Text = speedcntrlbar.Value
```

```
End Sub
```

```
Sub Stopbutton_Click ()
```

```
comd$ = "stop"
```

```
Rem
```

```
Call talking(comd$)
```

```
End Sub
```

```
Sub stopcntrloption_Click ()
```

```
comd$ = "stop1"
```

```
Call talking(comd$)
```

```
End Sub
```

ABOUT.FRM

VERSION 2.00

Begin Form ABOUT

```
Caption      = "About"
```

```
Height       = 3645
```

```
Left         = 1035
```

```
LinkTopic    = "Form2"
```

```
ScaleHeight   = 3120
```

```
ScaleWidth    = 3285
```

```
Top           = 1020
```

```
Width         = 3405
```

Begin CommandButton aboutexitbutton

```
Caption      = "Exit"
```

```
Height       = 495
```

```
Left         = 960
```

```
TabIndex     = 5
```

```
Top           = 2520
```

```
Width         = 1215
```

End

Begin Label progdatelabel

```
Alignment     = 2 'Center
```

```
Caption       = "February 1993"
```

```
Height        = 495
```

```
Left          = 960
```

```
TabIndex      = 4
```

```
Top            = 2040
```

```
Width          = 1215
```

End

Begin Label author2label

```
Alignment     = 2 'Center
```

```
Caption       = "Larry W. Jennings"
```

```

Height      = 255
Left        = 600
TabIndex    = 3
Top         = 1560
Width       = 1815
End
Begin Label andlabel
Alignment   = 2 'Center
Caption     = "and"
Height      = 255
Left        = 960
TabIndex    = 2
Top         = 1200
Width       = 1215
End
Begin Label author1label
Alignment   = 2 'Center
Caption     = "Alan C. Ewing"
Height      = 255
Left        = 600
TabIndex    = 1
Top         = 840
Width       = 1935
End
Begin Label progranamelabel
Alignment   = 2 'Center
Caption     = "TDL/Heliostat Control Program by:"
Height      = 495
Left        = 600
TabIndex    = 0
Top         = 240
Width       = 1935
End
End
Sub aboutexitbutton_Click ()
about.Hide

End Sub

```

Appendix C

The following table lists preliminary data results for the intensity measurements of methyl cyanide using the TDL spectrometer at the University of Tennessee Molecular Spectroscopy Laboratory. A 210 liter volume white cell using an 8.25 meter path length was used as the sample cell.

Table C.1

Methyl Cyanide TDL Absorption Spectrum Preliminary Data Results

ν_0 (cm^{-1})	Scans	Equivalent Width (cm^{-1})	HWHM (cm^{-1})	τ	Pressure (mTorr)	Temp. (K)	Doppler Width (cm^{-1})	Strength (HWHM) $\text{cm}^{-2} \text{ atm}^{-1}$	Strength (E. W.) $\text{cm}^{-2} \text{ atm}^{-1}$	% diff S(hwhm) & S(E.W.)
947.8774	105	1.0549E-04	1.0241E-03	0.9525	350	296	9.1205E-04	2.787E-04	2.8290E-04	-1.49
948.0760	105	1.2314E-04	1.0259E-03	0.9445	350	296	9.1215E-04	3.282E-04	3.3034E-04	-0.65
948.5201	105	7.0716E-05	1.1159E-03	0.9625	350	296	9.1263E-04	2.388E-04	1.8963E-04	22.96
948.9569	105	9.1230E-05	9.2945E-04	0.94661	350	296	9.1311E-04	2.857E-04	2.4465E-04	15.48
949.1449	105	2.0089E-04	1.0194E-03	0.91060	350	296	9.1320E-04	5.349E-04	5.3875E-04	-0.71
949.1449	35	1.9182E-04	1.0459E-03	0.91218	350	296	9.1320E-04	5.3868E-04	5.1439E-04	4.61
949.1449	105	7.8172E-05	1.0328E-03	0.95888	150	296	9.1320E-04	5.669E-04	4.8912E-04	14.74
949.1449	10	8.1872E-05	1.0225E-03	0.94444	150	296	9.1320E-04	7.641E-04	5.1227E-04	39.46
949.1449	105	2.0451E-04	1.0951E-03	0.91241	350	296	9.1320E-04	5.625E-04	5.4846E-04	2.53
1010.332	105	2.1243E-04	1.4059E-03	0.92620	120	296	9.7211E-04	1.761E-03	1.6616E-03	5.83
1010.332	10	2.4127E-04	1.3404E-03	0.91699	120	296	9.7211E-04	1.898E-03	1.8871E-03	0.58
1010.332	105	3.4669E-04	1.5432E-03	0.90296	220	296.5	9.7293E-04	1.404E-03	1.4791E-03	-5.20
1010.332	105	3.4730E-04	1.5187E-03	0.90184	220	296.5	9.7293E-04	1.398E-03	1.4818E-03	-5.77
1010.332	5	4.7294E-04	1.4200E-03	0.8744	220	296.5	9.7293E-04	1.698E-03	2.0177E-03	-17.17
1010.332	105	3.2164E-04	1.6808E-03	0.91422	180	296.5	9.7293E-04	1.642E-03	1.6770E-03	-2.09
1010.465	10	3.7377E-04	1.5304E-03	0.8964	120	296	9.7224E-04	2.733E-03	2.9234E-03	-6.71
1010.465	20	2.0465E-04	1.5159E-03	0.94051	61	296	9.7224E-04	2.988E-03	3.1487E-03	-5.21
1010.549	20	2.1324E-04	1.2954E-03	0.92210	61	296	9.7233E-04	3.377E-03	3.2811E-03	2.89
1010.549	10	6.5483E-04	2.0198E-03	0.86156	120	296	9.7233E-04	4.918E-03	5.1221E-03	-4.05

Appendix D

The following table lists preliminary results from the ethylene TDL absorption data. A 48.26 cm sample cell was used to take the absorption spectra. $\langle S \rangle$ is the average value of the strength (hwhm & τ) and strength (E.W.).

Table D.1

Ethylene TDL Absorption Spectrum Preliminary Data Results

ν_0 (cm ⁻¹)	Scans	Equivalent Width (cm ⁻¹)	HWHM (cm ⁻¹)	Tau	Pressure (mTorr)	Temp. (K)	Doppler Width (cm ⁻¹)	Strength (hwhm & τ) (cm ⁻² atm ⁻¹)	Strength (E.W.) (cm ⁻² atm ⁻¹)	$\langle S \rangle$ (cm ⁻² atm ⁻¹)	$\frac{\Delta S}{\langle S \rangle}$
941.8478	100	1.086E-03	1.166E-03	0.590	25	298.9	1.102E-03	0.8241	0.8247	0.8244	-0.0007
941.8478	100	1.089E-03	1.117E-03	0.584	25	299.4	1.103E-03	0.8070	0.8274	0.8172	-0.0250
941.8478	130	1.089E-03	1.167E-03	0.596	25	299.4	1.103E-03	0.8094	0.8278	0.8186	-0.0225
941.8478	100	6.539E-04	1.178E-03	0.735	15	299.8	1.104E-03	0.8103	0.7635	0.7869	0.0595
941.8478	75	7.0297E-04	1.199E-03	0.738	15	299.8	1.104E-03	0.8131	0.8279	0.8205	-0.0180
942.1013	100	6.865E-04	1.185E-03	0.739	100.3	298.6	1.102E-03	0.1196	0.1206	0.1201	-0.0083
942.1013	50	7.427E-04	1.199E-03	0.722	100.3	298.6	1.102E-03	0.1307	0.1318	0.1313	-0.0084
942.1013	20	7.429E-04	1.186E-03	0.708	100.3	298.6	1.102E-03	0.1368	0.1318	0.1343	0.0372
942.1013	100	6.563E-04	1.218E-03	0.746	100.3	298.6	1.102E-03	0.1194	0.1155	0.1175	0.0332
946.6999	100	1.774E-03	1.206E-03	0.421	100.3	297.9	1.106E-03	0.3492	0.3920	0.3706	-0.1155
946.7608	100	8.293E-04	1.165E-03	0.711	100.3	297.9	1.106E-03	0.1329	0.1494	0.1412	-0.1169
951.3701	100	1.981E-03	1.191E-03	0.330	33	296.6	1.109E-03	1.3099	1.401	1.3555	-0.0672
951.3701	75	1.402E-03	1.161E-03	0.505	20	296.6	1.109E-03	1.3302	1.4198	1.3750	-0.0652
951.3701	20	1.353E-03	1.153E-03	0.499	20	296.6	1.109E-03	1.3427	1.3549	1.3488	-0.0090
951.3702	100	1.975E-03	1.186E-03	0.338	33	296.6	1.109E-03	1.3072	1.388	1.3476	-0.0600
951.7379	5	9.476E-04	1.152E-03	0.651	32	296	1.108E-03	0.5173	0.5832	0.5503	-0.1198
951.7379	10	8.983E-04	1.191E-03	0.667	32	296	1.108E-03	0.5048	0.5479	0.5264	-0.0819
951.7379	20	8.723E-04	1.157E-03	0.668	32	296	1.108E-03	0.4895	0.5294	0.5095	-0.0783
951.7379	2	9.108E-04	1.176E-03	0.665	32	296	1.108E-03	0.5028	0.5568	0.5298	-0.1019
951.7379	20	5.771E-04	1.165E-03	0.778	20	296.6	1.109E-03	0.4899	0.4984	0.4942	-0.0172
951.7379	50	5.683E-04	1.133E-03	0.776	20	296.6	1.109E-03	0.4816	0.49	0.4858	-0.0173
951.7379	1	9.161E-04	9.933E-04	0.631	32	296	1.108E-03	0.4789	0.5606	0.5198	-0.1572
951.7379	500	8.637E-04	1.138E-03	0.667	32	296	1.108E-03	0.4832	0.5234	0.5033	-0.0799
951.7379	1000	8.530E-04	1.150E-03	0.671	32	296	1.108E-03	0.4807	0.4836	0.4822	-0.0060
951.7379	160	8.642E-04	1.140E-03	0.666	32	296	1.108E-03	0.4863	0.5237	0.5050	-0.0741
951.7379	40	8.472E-04	1.137E-03	0.668	32	296	1.108E-03	0.4809	0.5118	0.4964	-0.0623
951.7379	80	8.865E-04	1.127E-03	0.662	32	296	1.108E-03	0.4862	0.5394	0.5128	-0.1037
969.8509	50	4.277E-04	1.242E-03	0.848	25	299.4	1.136E-03	0.2738	0.2895	0.2817	-0.0557
969.8509	100	4.188E-04	1.317E-03	0.854	25	299.4	1.136E-03	0.2789	0.2836	0.2813	-0.0167
970.0230	100	6.537E-04	1.168E-03	0.750	25	299.7	1.137E-03	0.4506	0.4564	0.4535	-0.0128
970.0230	50	5.770E-04	1.200E-03	0.793	20	298.2	1.134E-03	0.4660	0.4973	0.4817	-0.0650

Table D.1 (cont.)

Ethylene TDL Absorption Spectrum Preliminary Data Results

ν_0 (cm^{-1})	Scans	Equivalent Width (cm^{-1})	HWHM (cm^{-1})	Tau	Pressure (mTorr)	Temp. (K)	Doppler Width (cm^{-1})	Strength (hwhm & τ) ($\text{cm}^{-2} \text{ atm}^{-1}$)	Strength (E.W.) ($\text{cm}^{-2} \text{ atm}^{-1}$)	$\langle S \rangle$ ($\text{cm}^{-2} \text{ atm}^{-1}$)	$\frac{\Delta S}{\langle S \rangle}$
970.0230	100	5.193E-04	1.150E-03	0.792	20	298.2	1.134E-03	0.4502	0.4433	0.4468	0.0154
970.0230	500	6.746E-04	1.192E-03	0.748	25	299.7	1.137E-03	0.4641	0.4727	0.4684	-0.0184
970.0230	20	7.242E-04	1.218E-03	0.745	25	299.7	1.136E-03	0.4806	0.5117	0.4962	-0.0627
1011.600	50	2.281E-04	1.324E-03	0.917	25	299.4	1.184E-03	0.1532	0.1523	0.1528	0.0059
1011.600	50	2.232E-04	1.324E-03	0.926	25	299.4	1.184E-03	0.1364	0.1478	0.1421	-0.0802

Appendix E

The following table lists absorption line strengths from the ν_7 band of ethylene. Data were supplied by John Hillman of GSFC and KPNO Fourier Transform Spectrometer. Strengths were measured using Dr. Mark Weber's fitting programs and the strength values have been corrected to TDL values using calibration in Chapter 3 and scaled to 296K.

Table E.1

Ethylene Absorption Line Strengths from FTS Data

J'	Ka'	Kc'	J''	Ka''	Kc''	Frequency (cm ⁻¹)	Strength (cm ⁻² atm ⁻¹)
11	1	10	11	2	10	941.84782	0.8240
19	4	16	20	3	18	942.04403	0.14572
8	2	6	9	1	8	942.10127	0.1157
11	3	9	10	4	7	942.53144	0.15636
12	1	11	12	2	11	942.59618	0.36441
5	1	4	6	0	6	943.43526	0.29320
24	2	22	24	3	22	943.98244	0.10431
14	1	13	14	2	13	944.10129	0.39552
7	2	5	8	1	7	944.22741	0.10665
11	3	8	12	2	10	944.66893	0.18149
14	3	12	15	2	14	944.79754	0.13536
15	1	14	15	2	14	944.82451	0.87549
1	0	1	1	1	1	944.90301	0.12790
4	0	4	4	1	4	945.58181	0.37978
5	0	5	5	1	5	945.91746	0.47624
3	1	2	4	0	4	946.11957	0.2400
17	1	16	17	2	16	946.13449	0.84359
6	1	6	5	2	4	946.17457	0.1210
6	0	6	6	1	6	946.28257	0.5699
6	2	4	7	1	6	946.42473	0.09420
7	0	7	7	1	7	946.65922	0.63645
13	3	10	12	4	8	946.76234	0.1461
9	2	7	8	3	5	947.01202	0.08196
10	2	9	11	1	11	947.06304	0.06942
16	4	13	17	3	15	947.09606	0.07029
10	2	9	9	3	7	947.13905	0.08216
19	1	18	19	2	18	947.19850	0.75356
9	0	9	9	1	9	947.38063	0.74253

Table E.1 (cont.)

Ethylene Absorption Line Strengths from FTS Data

J'	Ka'	Kc'	J''	Ka''	Kc''	Frequency (cm ⁻¹)	Strength (cm ⁻² atm ⁻¹)
9	0	9	9	1	9	947.38064	0.74434
12	3	10	13	2	12	947.45354	0.16238
20	1	19	20	2	19	947.63118	0.29879
10	0	10	10	1	10	947.70017	0.79050
11	0	11	11	1	11	947.98289	0.85493
21	1	20	21	2	20	948.00199	0.64865
12	1	12	12	0	12	948.22772	0.89827
22	1	21	22	2	21	948.31790	0.23345
8	1	8	7	2	6	948.44911	0.17450
23	1	22	23	2	22	948.58651	0.48595
15	0	15	15	1	15	948.76356	0.78524
16	0	16	16	1	16	948.89291	0.73873
17	0	17	17	1	17	949.00611	0.70354
18	1	18	18	0	18	949.10736	0.63138
20	1	20	20	0	20	949.41389	1.18843
24	2	23	24	1	23	949.75582	0.20434
11	1	11	11	0	11	949.83054	0.93518
21	2	20	21	1	20	950.13674	0.30552
30	1	30	30	0	30	950.17644	0.24051
9	1	9	9	0	9	950.33119	0.77197
20	2	19	20	1	19	950.38050	0.31633
19	2	18	19	1	18	950.69592	0.33250
18	2	17	18	1	17	951.06147	0.31611
16	2	14	15	4	12	951.23002	0.14107
6	1	6	6	0	6	951.37167	1.4155
6	2	4	7	1	6	951.58102	0.22372
17	1	16	17	2	16	951.60759	0.37152
26	2	24	26	3	24	951.65265	0.16531
5	1	5	5	0	5	951.73936	0.47778
3	1	3	3	0	3	952.38591	0.31559
3	1	3	3	0	3	952.62780	0.50591
1	1	1	1	0	1	952.79636	0.13361
3	2	1	4	1	3	953.09905	0.09682
14	2	13	14	1	13	953.53061	0.40410
8	1	7	7	2	5	953.66833	0.11558
8	3	6	9	2	8	953.72539	0.15404
16	1	16	15	2	14	953.87908	0.11206
6	0	6	5	1	4	954.10416	0.13616
13	2	12	13	1	12	954.29327	0.40343
18	3	16	17	4	14	954.43783	0.13516
1	1	0	0	0	0	954.79086	0.21958

Table E.1 (cont.)

Ethylene Absorption Line Strengths from FTS Data

J'	Ka'	Kc'	J''	Ka''	Kc''	Frequency (cm ⁻¹)	Strength (cm ⁻² atm ⁻¹)
7	0	7	6	1	5	955.16688	0.14649
17	3	14	16	4	12	955.57585	0.14950
9	1	8	8	2	3	955.67201	0.34793
11	2	10	11	1	10	955.88598	0.36880
8	0	8	7	1	6	956.05196	0.14388
10	2	9	10	1	9	956.67564	0.36394
2	1	1	1	0	1	956.77624	0.13815
10	0	10	9	1	8	957.26356	0.11528
20	3	18	19	4	16	957.39144	0.10954
10	1	9	9	2	7	957.56088	0.15826
14	2	12	13	3	10	958.57194	0.11726
3	1	2	2	0	2	958.84222	0.39942

VITA

Larry Wayne Jennings was born in Kingsport, Tennessee on October 28, 1964. He grew up in Gate City, Virginia and attended public school there. He graduated from Gate City High School in May, 1983. He began his college education at the Mountain Empire Community College in January, 1983 and received an Associate Degree in Applied Science with a major in Electronics in May, 1985. He entered King College in Bristol, Tennessee in the fall of 1986 and conducted research in Astronomy while there. He received a Bachelor of Science degree in Physics in May, 1988. The following fall, he began graduate studies at the University of Tennessee with a teaching assistantship and later a research assistantship at the Oak Ridge National Laboratory. He received his Master of Science degree in Physics with a concentration in Molecular Spectroscopy in December, 1994.