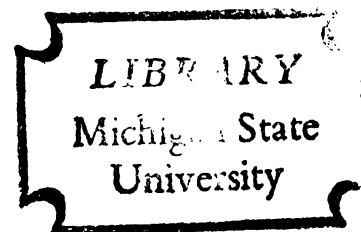


HIGH RESOLUTION ABSORPTION, ZEEMAN AND
MAGNETIC ROTATION SPECTRA OF THE FUNDAMENTAL
AND SATELLITE BANDS OF NITRIC OXIDE IN THE
NEAR INFRARED

Thesis for the Degree of Ph. D.
MICHIGAN STATE UNIVERSITY
DONALD B. KECK

1967



This is to certify that the

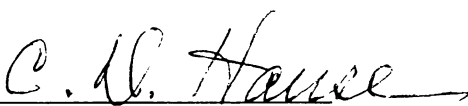
thesis entitled

HIGH RESOLUTION ABSORPTION, ZEEMAN
AND MAGNETIC ROTATION SPECTRA OF
THE FUNDAMENTAL AND SATELLITE
BANDS OF NITRIC OXIDE IN
THE NEAR INFRARED
presented by

Donald B. Keck

has been accepted towards fulfillment
of the requirements for

Ph. D. degree in Physics


Major professor

Date November 17, 1967





ABSTRACT

HIGH RESOLUTION ABSORPTION, ZEEMAN AND MAGNETIC ROTATION SPECTRA OF THE FUNDAMENTAL AND SATELLITE BANDS OF NITRIC OXIDE IN THE NEAR INFRARED

by Donald B. Keck

The absorption, Zeeman and magnetic rotation spectra of the 1-0 vibration-rotation bands of nitric oxide have been obtained using the Michigan State University high resolution ($\sim 0.07 \text{ cm}^{-1}$ at $\sim 2000 \text{ cm}^{-1}$) near infrared spectrometer. This included the weak satellite transitions, $^2\Pi_{1/2} \rightarrow ^2\Pi_{3/2}$ and $^2\Pi_{3/2} \rightarrow ^2\Pi_{1/2}$. Improved values of the molecular constants have been obtained by a simultaneous least squares analysis of combination differences and frequencies. The spin-orbit constant was determined directly by means of the satellite band frequencies which were included.

Theoretical calculations of the Zeeman patterns and intensities have been given. The observed spectra match these predictions very closely.

A phenomenological theory of magnetic rotation spectra is outlined. Predictions made on the basis of this theory explain the major features of the observed magnetic rotation signals starting from rather basic principles. These features include the doublet structure of lines at high pressure and the intensity contour of the 2-subband.

ABSTRACT

HIGH RESOLUTION ABSORPTION, ZEEMAN AND MAGNETIC ROTATION SPECTRA OF THE FUNDAMENTAL AND SATELLITE BANDS OF NITRIC OXIDE IN THE NEAR INFRARED

by Donald B. Keck

The absorption, Zeeman and magnetic rotation spectra of the 1-0 vibration-rotation bands of nitric oxide have been obtained using the Michigan State University high resolution ($\sim 0.07 \text{ cm}^{-1}$ at $\sim 2000 \text{ cm}^{-1}$) near infrared spectrometer. This included the weak satellite transitions, $^2\Pi_{1/2} \rightarrow ^2\Pi_{3/2}$ and $^2\Pi_{3/2} \rightarrow ^2\Pi_{1/2}$. Improved values of the molecular constants have been obtained by a simultaneous least squares analysis of combination differences and frequencies. The spin-orbit constant was determined directly by means of the satellite band frequencies which were included.

Theoretical calculations of the Zeeman patterns and intensities have been given. The observed spectra match these predictions very closely.

A phenomenological theory of magnetic rotation spectra is outlined. Predictions made on the basis of this theory explain the major features of the observed magnetic rotation signals starting from rather basic principles. These features include the doublet structure of lines at high pressure and the intensity contour of the 2-subband.

Donald B. Keck

Modifications made in the above mentioned instrument are discussed. These include a rod source, a vacuum polarizer assembly, new monochromator mirrors, a new grating drive assembly, and new detectors. All air paths in the entire optical train have been eliminated.

HIGH RESOLUTION ABSORPTION, ZEEMAN AND MAGNETIC ROTATION
SPECTRA OF THE FUNDAMENTAL AND SATELLITE BANDS
OF NITRIC OXIDE IN THE NEAR INFRARED

By

Donald B. Keck

A THESIS

Submitted to
Michigan State University
in partial fulfillment of the requirements
for the degree of

DOCTOR OF PHILOSOPHY

Department of Physics

1967

ACKNOWLEDGEMENTS

I am very grateful to Professor C. D. Hause for his help and guidance throughout my work. I have considered it a privilege to work and learn under him. It was he who suggested this problem and encouraged me throughout the research. I owe a special thanks to Professor T. H. Edwards. He too has given much helpful advice and assistance during all phases of this work. I wish to thank Professors P. M. Parker, R. D. Spence and J. A. Cowen. All presented excellent courses and have been helpful with many questions.

I wish to thank former graduate students, Drs. Joseph Aubel and Melvin Olman for their friendship and assistance. Dr. Aubel was an excellent teacher concerning the spectrometer and the magnetic rotation work. Dr. Olman was very helpful with the modifications of the instrument, the computer work and the analysis.

I am also indebted to former graduate students, Drs. Jerry Johnston, Kent Moncur, Tom Barnett and Lew Snyder for their friendship and many discussions.

The friendship of my fellow graduate students Lamar "Dutch" Bullock, Pete Willson, Dick Blank and Dick Peterson is greatly appreciated. A special thanks is extended to Dutch Bullock for his collaboration on several projects.

I wish to thank the National Science Foundation for their generous support of this work through various grants and fellowships. The M. S. U. Computer Center has also been very helpful in this work.

I want to take this opportunity to thank my father, Dr. W. G. Keck, for all the valuable guidance and training he has given me which stood me in good stead for this work.

Finally, but by no means least, I want to thank my wife Ruth for her encouragement throughout this work and the many hours she spent in the preparation of this thesis.

TABLE OF CONTENTS

	Page
ACKNOWLEDGEMENTS.	ii
LIST OF TABLES.	v
LIST OF FIGURES	vi
LIST OF APPENDICES.	viii
INTRODUCTION.	1
Chapter	
1 ROTATION-VIBRATION ENERGY FOR AN INTERMEDIATE $^2\Pi$ STATE.	4
2 WAVEFUNCTIONS AND INTENSITIES.	13
3 ZEEMAN ENERGIES.	26
4 MAGNETIC ROTATION THEORY	29
5 ABSORPTION ANALYSIS.	36
6 ZEEMAN ANALYSIS.	53
7 MAGNETIC ROTATION ANALYSIS	57
8 SPECTROMETER DESCRIPTION	81
SUMMARY	104
REFERENCES.	105
APPENDICES.	110

LIST OF TABLES

Table	Page
1.1 Matrix of H'_r in Pure Case (a) Basis.	7
1.2 Matrix of $H'_r + A(\vec{L} \cdot \vec{S})$ in Symmetrized Case (a) Basis	7
1.3 Matrix of $H'_r + A(\vec{L} \cdot \vec{S})$	7
2.1 Direction Cosine Matrix Elements	18
5.1 Experimental Conditions for Absorption Spectra . . .	37
5.2 Effective Constants for NO	44
5.3 Comparison of Effective Constants for NO	46
5.4 Rotational Constants for NO.	47
5.5 Spin-Orbit Constants for NO.	48
5.6 Isotopic Calculations for $^{15}\text{N}^{16}\text{O}$	48
6.1 Zeeman Splittings for the $(1-0)$, $P_2(5/2)$ and $R_2(3/2)$ Lines of $^{14}\text{N}^{16}\text{O}$ and $^{15}\text{N}^{16}\text{O}$ as a Function of Field.	56
8.1 Spectrometer Optics.	87



LIST OF FIGURES

Figure		Page
5.1	High resolution spectra of the Q-branch region of the 1-0 HES band of $^{15}\text{N}^{16}\text{O}$	38
5.2	High resolution spectra of the Q-branch region of the 1-0 LES band of $^{15}\text{N}^{16}\text{O}$	39
6.1	a) Observed Zeeman spectra for the 1-0 band, $P_2(5/2)$ line of $^{14}\text{N}^{16}\text{O}$ as a function of field b) Predicted Zeeman spectra for the same conditions as in a)	54
7.1	Magnetic rotation spectra of the 1-0 band, P-branch of $^{14}\text{N}^{16}\text{O}$ as a function of pressure. . . .	58
7.2	Magnetic rotation spectra of the 1-0 band of $^{14}\text{N}^{16}\text{O}$ as a function of pathlength	59
7.3	Magnetic rotation spectra of the 1-0 band, P-branch of $^{14}\text{N}^{16}\text{O}$ as a function of field	60
7.4	Magnetic rotation spectra of the 1-0 band of $^{14}\text{N}^{16}\text{O}$ as a function of polarizer angle. . . .	61
7.5	Magnetic rotation spectra of the R-branch region of the 1-0 HES band of $^{14}\text{N}^{16}\text{O}$ as a function of field and pressure.	62
7.6	Predicted Zeeman patterns and relative intensities for the 1-0 band, P-branch of $^{14}\text{N}^{16}\text{O}$ for a magnetic field strength of 6000 gauss	65
7.7	Typical anomalous dispersion curves for a simple Zeeman doublet	66
7.8	Predictions of the terms making up the magnetic rotation signal of the 1-0 band, $P_1(15/2)$ line of $^{14}\text{N}^{16}\text{O}$	68
7.9a	Predictions of the magnetic rotation signal for the 1-0 band, $P_1(15/2)$ line at pressures of 1.0 and 10.3 torr.	72



Figure	Page
7.9b Predictions of the magnetic rotation signal for the 1-0 band, $P_2(15/2)$ line at pressures of 1.0 and 10.3 torr.	73
7.10 Predictions of the magnetic rotation signal for the 1-0 band, P_2 subband of $^{14}\text{N}^{16}\text{O}$ at pressures of 1.0 and 10.3 torr.	75
7.11 Predicted Zeeman patterns and relative intensities for the 1-0 HES band, R-branch of $^{14}\text{N}^{16}\text{O}$ for a field strength of 6000 gauss	78
8.1 Rod source.	83
8.2 Rod source power supply	84
8.3 Foreoptics, polarizer assembly and solenoid	86
8.4 Polarizer assembly.	90
8.5 Monochromator and exit optics	91
8.6 Grating drive train	96
8.7 Calibration system.	98



LIST OF APPENDICES

Appendix	Page
I A. Matrix elements of H_r^1	110
B. Matrix elements of $A(L \cdot \vec{S})$	111
II A. Intermediate wave functions for the v = 0 and v = 1 states of $^{14}\text{N}^{16}\text{O}$	112
B. Intermediate wave functions for the v = 0 and v = 1 states of $^{15}\text{N}^{16}\text{O}$	116
III A. Calculated line strengths for $^{14}\text{N}^{16}\text{O}$	120
B. Calculated line strengths for $^{15}\text{N}^{16}\text{O}$	123
IV Calculated values for the integrated absorption coefficients for $^{14}\text{N}^{16}\text{O}$	126
V A. g-factors for $^{14}\text{N}^{16}\text{O}$	131
B. g-factors for $^{15}\text{N}^{16}\text{O}$	133
VI Expressions used in the fitting programs	
A. Combination differences	135
B. Frequencies	135
C. Λ -doublet splittings.	137
VII Computer programs	
A. SHAFT	139
B. DIFF.	164
C. ROTCONS	176
D. ALLFIT.	176
E. LAMCON.	176
F. STEPFIT	176
G. ZEEPUN.	196
H. PLOTGUN	203
VIII A. GSCD and frequency fit (inputing constants from the GSCD fit) for $^{14}\text{N}^{16}\text{O}$	220
B. GSCD and frequency fit (inputing constants from the GSCD fit) for $^{15}\text{N}^{16}\text{O}$	228
IX A. Frequency fit for $^{14}\text{N}^{16}\text{O}$	235
B. Frequency fit for $^{15}\text{N}^{16}\text{O}$	240
X A. Λ -doublet splitting fit for $^{14}\text{N}^{16}\text{O}$	245
B. Λ -doublet splitting fit for $^{15}\text{N}^{16}\text{O}$	248



INTRODUCTION

Nitric oxide, being the only stable diatomic molecule possessing an odd number of electrons and an electronic angular momentum, has been the subject of many investigations (1-16). The result is a $^2\Pi$ ground state whose components are separated by $\sim 120\text{ cm}^{-1}$ by a spin-orbit interaction. The coupling is intermediate between Hund's cases (a) and (b). In addition the intermediate coupling makes both Π states magnetically sensitive.

Improvements in infrared detectors since Shaw's (6) work on NO in 1956 has led to an increased interest in the vibration-rotation spectra of the fundamental region ($\sim 1900\text{ cm}^{-1}$).

This work has been concerned with obtaining and analyzing high resolution absorption, Zeeman and magnetic rotation spectra of both $^{14}\text{N}^{16}\text{O}$ and $^{15}\text{N}^{16}\text{O}$ for this region, including the weak satellite transitions, $^2\Pi_{1/2} \rightarrow ^2\Pi_{3/2}$ and $^2\Pi_{3/2} \rightarrow ^2\Pi_{1/2}$.

The system used in obtaining the spectra is described in Chapter 8. This includes an account of the modifications which were necessary to extend the range of the instrument to enable these spectra to be recorded.



Analysis of the absorption spectra was carried out using the existing theory (9, 17, 18, 19, 20) which is outlined in Chapter 1. A simultaneous analysis of all observed transitions for each isotope is carried out in Chapter 5 and leads to improved values of existing molecular constants through the use of least squares fits to both combination differences and frequencies. Inclusion of the satellite data provides a direct determination of the spin-orbit coupling constant and helps resolve previous differences regarding this quantity.

Zeeman components were resolved for two low J-value lines for both isotopes. The theory necessary to explain their positions and a brief analysis of them is given in Chapters 3 and 6 respectively.

In Chapter 2 the quantum mechanical theory for the intensities of the transitions is given. These calculations are necessary for the magnetic rotation analysis.

Buckingham and Stephens (21) have given a review of the theory for magnetic rotation spectra from a phenomenological viewpoint. A brief account of their approach and the deviations from it as proposed by Aubel (22) are given in Chapter 4. Aubel's approach coupled with the results of Chapter 2 enable theoretical predictions of the magnetic rotation signal to be made starting from rather basic principles. With the help of the computer these predictions have been made for several representative transitions and are given together with the observations in Chapter 7.



It is found that the major features of the observed signal can be explained by this theory on a semi-quantitative level.



CHAPTER 1

ROTATION-VIBRATION ENERGY FOR AN INTERMEDIATE $^2\Pi$ STATE

The molecular Hamiltonian of a diatomic molecule, for the region of spectrum being considered here, can be written (23) as a sum of an electronic, a vibrational, and a rotational term, viz.

$$H = H_e + H_v + H_r . \quad (1.1)$$

Vibrational Term

Assuming an anharmonic oscillator as a model, the form for the vibrational energy has long been known. Herzberg (24) gives the term value as:

$$G(v) = \omega_e(v+\frac{1}{2}) - \omega_e x_e(v+\frac{1}{2})^2 + \omega_e y_e(v+\frac{1}{2})^3 + \dots . \quad (1.2)$$

where $G(v)$ is in cm^{-1} , v is the vibrational quantum number and $\omega_e \gg \omega_e x_e \gg \omega_e y_e$ are vibrational constants.

Rotational Term

Here the pure end over end rotation of the molecule is considered. If J is the total angular momentum quantum number in units of $\hbar$, and assuming the possibility of orbital, L , and spin, S , electronic angular momenta, the end over end rotational angular momentum of the molecule is:

$$\vec{P} = \vec{J} - \vec{L} - \vec{S} \quad . \quad (1.3)$$

For the case of the diatomic molecule, taking the body fixed z-direction along the internuclear axis, $P_z = 0$ so that:

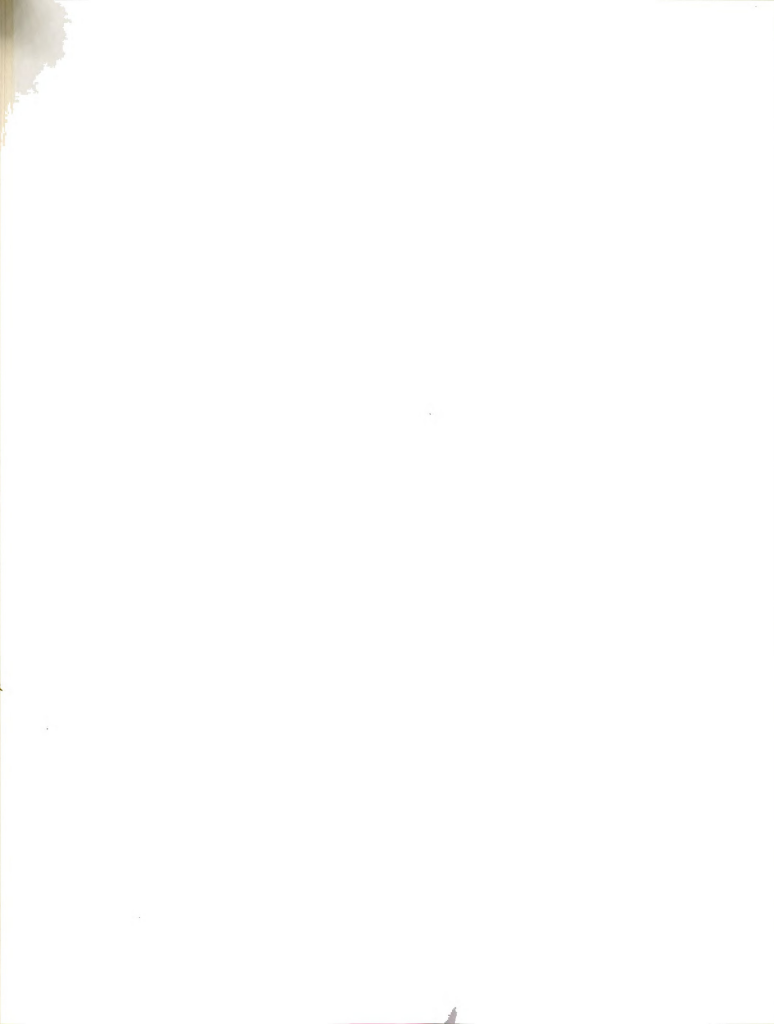
$$\begin{aligned} H_r' &= BP^2 = B[(J_x - L_x - S_x)^2 + (J_y - L_y - S_y)^2] \\ &= B[J^2 - L^2 + S^2 - 2\vec{J} \cdot \vec{S} + L^2 - \Lambda^2] \\ &\quad + 2B[(L_x S_x + L_y S_y) - (J_x L_x + J_y L_y)] \quad , \quad (1.4) \end{aligned}$$

where B is the rotational constant.

The matrix elements for the Hamiltonian in equation (1.4) have been given by Van Vleck (18) and later by Dousmanis, Sanders and Townes (20) for a pure Hund's case (a) coupling scheme. These are listed in Appendix I-A with their phase conventions. In this representation both L and S are quantized along the internuclear axis with the eigenvalues Λ and Σ respectively. Herzberg (25) discusses this and other coupling schemes in detail. The total angular momentum along the axis is designated by $\Omega = |\Lambda + \Sigma|$.

For the case of NO or any other molecule with an unpaired p-electron, $L = 1$, its projection $\Lambda = 0, \pm 1$, $S = \frac{1}{2}$ and its projection $\Sigma = \pm \frac{1}{2}$. With these quantum numbers six case (a) states can be formed with the designation $^{2S+1}|\Lambda|_{\Lambda+\Sigma}$ viz.

$$^2\Pi_{\frac{1}{2}}, \quad ^2\Pi_{-\frac{1}{2}}, \quad ^2\Pi_{\frac{3}{2}}, \quad ^2\Pi_{-\frac{3}{2}}, \quad ^2\Sigma_{\frac{1}{2}}, \quad ^2\Sigma_{-\frac{1}{2}} \quad .$$



$$\vec{P} = \vec{J} - \vec{L} - \vec{S} \quad . \quad (1.3)$$

For the case of the diatomic molecule, taking the body fixed z-direction along the internuclear axis, $P_z = 0$ so that:

$$\begin{aligned} H'_r &= BP^2 = B[(J_x - L_x - S_x)^2 + (J_y - L_y - S_y)^2] \\ &= B[J^2 - L^2 + S^2 - 2\vec{J} \cdot \vec{S} + L^2 - \Lambda^2] \\ &\quad + 2B[(L_x S_x + L_y S_y) - (J_x L_x + J_y L_y)] \quad , \quad (1.4) \end{aligned}$$

where B is the rotational constant.

The matrix elements for the Hamiltonian in equation (1.4) have been given by Van Vleck (18) and later by Dousmanis, Sanders and Townes (20) for a pure Hund's case (a) coupling scheme. These are listed in Appendix I-A with their phase conventions. In this representation both L and S are quantized along the internuclear axis with the eigenvalues Λ and Σ respectively. Herzberg (25) discusses this and other coupling schemes in detail. The total angular momentum along the axis is designated by $\Omega = |\Lambda + \Sigma|$.

For the case of NO or any other molecule with an unpaired p-electron, $L = 1$, its projection $\Lambda = 0, \pm 1$, $S = \frac{1}{2}$ and its projection $\Sigma = \pm \frac{1}{2}$. With these quantum numbers six case (a) states can be formed with the designation $^{2S+1}|\Lambda|_{\Lambda+\Sigma}$ viz.

$$^2\Pi_{\frac{1}{2}}, \quad ^2\Pi_{-\frac{1}{2}}, \quad ^2\Pi_{\frac{3}{2}}, \quad ^2\Pi_{-\frac{3}{2}}, \quad ^2\Sigma_{\frac{1}{2}}, \quad ^2\Sigma_{-\frac{1}{2}} \quad .$$

The interactions of these six states form a 6×6 matrix, as given in Table 1.1. This matrix can be factored by choosing as a basis, symmetric and antisymmetric combinations first proposed by Kronig (26), of the six pure case (a) wave functions, viz.

$$\psi(\Lambda, \Sigma, \Omega)_{s,a} = \frac{1}{\sqrt{2}} [\psi(\Lambda, \Sigma, \Omega) \pm \psi(-\Lambda, -\Sigma, -\Omega)] \quad (1.5)$$

This factorization breaks the Hamiltonian matrix into two 3×3 blocks of opposite parity, similar to that shown in Table 1.2. The eigenvalues of the symmetric (antisymmetric) block corresponds to the c(d) level (Λ -doublet levels) of Mulliken (27). The only difference between the two blocks is in the Σ - Σ and the Σ - $\Pi_{\frac{1}{2}}$ terms. These matrix elements stem from the last line of equation (1.4) which is off diagonal in Λ . The degeneracy in Λ is lifted by the interaction of the Π with the nearby Σ state. Similar terms will enter when the spin-orbit interaction is considered.

Electronic Term

For this work only the ground electronic state need be considered. Its energy may be taken as some constant, T_e . An additional energy will arise when the electronic orbital and spin angular momentum interaction is included. The total electronic energy can therefore be written:

$$H_e = T_e + A(\vec{L} \cdot \vec{S}) \quad (1.6)$$

Table 1.1 Matrix of H'_r in Pure Case (a) Basis.

$$H'_r = \begin{matrix} & \begin{matrix} \Sigma_{\frac{1}{2}} & \Pi_{\frac{1}{2}} & \Pi_{\frac{3}{2}} & \Sigma_{-\frac{1}{2}} & \Pi_{-\frac{1}{2}} & \Pi_{-\frac{3}{2}} \end{matrix} \\ \begin{matrix} \alpha & \theta_1 & \eta & \delta & \zeta & 0 \\ \theta_1^* & \beta_1 & \epsilon & \zeta & 0 & 0 \\ \eta^* & \epsilon^* & \gamma_1 & 0 & 0 & 0 \\ \delta^* & \zeta^* & 0 & \alpha & \theta_1 & \eta \\ \zeta^* & 0 & 0 & \theta_1^* & \beta_1 & \epsilon \\ 0 & 0 & 0 & \eta^* & \epsilon^* & \gamma_1 \end{matrix} \end{matrix}$$

Table 1.2 Matrix of $H'_r + A(\vec{L} \cdot \vec{S})$ in Symmetrized Case ($\bar{a}$) Basis.

$$H'_r + A(\vec{L} \cdot \vec{S}) = \begin{matrix} & \begin{matrix} \Sigma_{\frac{1}{2}}^S & \Pi_{\frac{1}{2}}^S & \Pi_{\frac{3}{2}}^S & \Sigma_{\frac{1}{2}}^a & \Pi_{\frac{1}{2}}^a & \Pi_{\frac{3}{2}}^a \end{matrix} \\ \begin{matrix} \kappa^S & \mu^S & \eta & & & \\ (\mu^S)^* & \beta & \epsilon & & 0 & \\ \eta^* & \epsilon^* & \gamma & & & \\ & 0 & & \kappa^a & \mu^a & \eta \\ & & & (\mu^a)^* & \beta & \epsilon \\ & & & \eta^* & \epsilon^* & \gamma \end{matrix} \end{matrix}$$

Table 1.3 Matrix of $H'_r + A(\vec{L} \cdot \vec{S})$.

$$H'_r + A(\vec{L} \cdot \vec{S}) = \begin{matrix} & \Pi_{\frac{1}{2}} & \Pi_{\frac{3}{2}} \\ \begin{matrix} \beta + \rho^2(\beta_1^2 + \epsilon^2) & \epsilon[1 + \rho^2(\beta_1 + \gamma_1)] \\ \epsilon^*[1 + \rho^2(\beta_1 + \gamma_1)] & \gamma + \rho^2(\gamma_1^2 + \epsilon^2) \end{matrix} \end{matrix}$$

where $\rho = D^{\pi}/B^{\pi}$.

Table 1.1 Matrix of H_r^i in Pure Case (a) Basis.

$$H_r^i = \begin{matrix} & \Sigma_{\frac{1}{2}} & \Pi_{\frac{1}{2}} & \Pi_{\frac{3}{2}} & \Sigma_{-\frac{1}{2}} & \Pi_{-\frac{1}{2}} & \Pi_{-\frac{3}{2}} \\ \begin{pmatrix} \alpha & \theta_1 & \eta & \delta & \zeta & 0 \\ \theta_1^* & \beta_1 & \epsilon & \zeta & 0 & 0 \\ \eta^* & \epsilon^* & \gamma_1 & 0 & 0 & 0 \\ \delta^* & \zeta^* & 0 & \alpha & \theta_1 & \eta \\ \zeta^* & 0 & 0 & \theta_1^* & \beta_1 & \epsilon \\ 0 & 0 & 0 & \eta^* & \epsilon^* & \gamma_1 \end{pmatrix} \end{matrix}$$

Table 1.2 Matrix of $H_r^i + A(\vec{L} \cdot \vec{S})$ in Symmetrized Case ($\bar{a}$) Basis.

$$H_r^i + A(\vec{L} \cdot \vec{S}) = \begin{matrix} & \Sigma_{\frac{1}{2}}^S & \Pi_{\frac{1}{2}}^S & \Pi_{\frac{3}{2}}^S & \Sigma_{\frac{1}{2}}^a & \Pi_{\frac{1}{2}}^a & \Pi_{\frac{3}{2}}^a \\ \begin{pmatrix} \kappa^S & \mu^S & \eta & & & \\ (\mu^S)^* & \beta & \epsilon & & 0 & \\ \eta^* & \epsilon^* & \gamma & & & \\ & 0 & & \kappa^a & \mu^a & \eta \\ & & & (\mu^a)^* & \beta & \epsilon \\ & & & \eta^* & \epsilon^* & \gamma \end{pmatrix} \end{matrix}$$

Table 1.3 Matrix of $H_r^i + A(\vec{L} \cdot \vec{S})$.

$$H_r^i + A(\vec{L} \cdot \vec{S}) = \begin{matrix} & \Pi_{\frac{1}{2}} & \Pi_{\frac{3}{2}} \\ \begin{pmatrix} \beta + \rho^2(\beta_1^2 + \epsilon^2) & \epsilon[1 + \rho^2(\beta_1 + \gamma_1)] \\ \epsilon^*[1 + \rho^2(\beta_1 + \gamma_1)] & \gamma + \rho^2(\gamma_1^2 + \epsilon^2) \end{pmatrix} \end{matrix}$$

where $\rho \equiv D^{\pi}/B^{\pi}$.

Matrix elements of the spin-orbit Hamiltonian are given in Appendix I-B in the pure case (a) basis. In the symmetrized basis discussed above the matrix of $H_r' + A(\vec{L} \cdot \vec{S})$ is given in Table 1.2.

Diagonalization of H_e and H_r

At this point the two 3×3 subblocks of Table 1.2, obtained by adding $H_e + H_r'$, may be diagonalized to obtain rotational and electronic eigenvalues. Dousmanis, Sanders and Townes (20) have shown that by diagonalizing to successively higher orders in $(E_{elec})^{-1}$ the problem reduces to diagonalizing the 2×2 submatrix:

$$\begin{pmatrix} \beta & \epsilon \\ \epsilon^* & \gamma \end{pmatrix} \quad (1.7)$$

This is acceptable for the case of NO since it is known that the ground state is the $^2\Pi$ and $E_{\pi-\pi}$ is $\sim 120 \text{ cm}^{-1}$ and $E_{\Sigma-\pi}$ is $\sim 32,000 \text{ cm}^{-1}$. Terms in $1/E_{\Sigma-\pi}$ will therefore be small. It is seen that to this order the eigenvalues for the symmetric and antisymmetric blocks are equal.

These eigenvalues are:

$$\begin{aligned} E_{1,2} &= \frac{1}{2}(\beta + \gamma) \pm \frac{1}{2}[(\beta - \gamma)^2 + 4|\epsilon|^2]^{\frac{1}{2}} \\ &= \frac{1}{2}(\beta + \gamma) \pm \frac{1}{2}B^{\pi}X \end{aligned} \quad (1.8)$$

where

$$X = [4(J + \frac{1}{2})^2 + \lambda(\lambda - 4)]^{\frac{1}{2}}; \quad \lambda = A/B^{\pi}$$

Here the upper (lower) sign is used with E_1 (E_2) where this energy corresponds to an intermediate ${}^2\Pi_{1/2}$ (${}^2\Pi_{3/2}$) state. These energies were first given by Hill and Van Vleck (17) starting from pure case (b) wave functions. Van Vleck (18) later obtained the same answer starting from pure case (a) wave functions as was outlined here.

Centrifugal Distortion

Thus far our model for rotation has been that of a rigid rotator. To account for non-rigidity a term must be added to H_r which varies as P^4 . A term of this form was added by Almy and Horsfall (19). Their Hamiltonian including the spin-orbit term is:

$$H_r = BP^2 - DP^4 + A(\vec{L} \cdot \vec{S}) \quad , \quad (1.9)$$

where D is the centrifugal distortion constant. Finally, considering matrix elements in the symmetrized basis which only involve the Π states, as was done in Eq. (1.7), this Hamiltonian matrix is as given in Table 1.3. This matrix can be diagonalized with the result that:

$$\begin{aligned} E_{1,2} = & B^\pi [(J+\tfrac{1}{2})^2 - \Lambda^2] + B^\pi [L(L+1) - \Lambda^2] \\ & \pm [\tfrac{1}{4}A(A - 4B^\pi)\Lambda^2 + B^{\pi 2}(J+\tfrac{1}{2})^2]^{\frac{1}{2}} \\ & - D^\pi [J^2(J+1)^2 - \tfrac{1}{2}J(J+1) + \tfrac{1}{16}] \quad . \end{aligned} \quad (1.10)$$

In this expression terms of order D^π/B^π have been omitted. The term $L^2 - \Lambda^2$ was also omitted in the P^4 term.

Vibration-Rotation Interactions

To this point the vibration and rotation of the molecule have been considered as independent motions. It is reasonable to assume that the rotational constants considered so far are really time averages over the period of vibration. It is also reasonable that, because of the anharmonicity, the average separation will increase with increasing vibrational quantum numbers. The rotational constant, B , which varies as r^{-2} will be a decreasing function of v . From rather involved calculations (for a simple example, see Pauling and Wilson (28)) the rotational constants are given by:

$$B_v = B_e - \alpha_e (v + \frac{1}{2}) \quad (1.11)$$

$$D_v = D_e + \beta_e (v + \frac{1}{2}) \quad , \quad (1.12)$$

where α_e and β_e are the vibration-rotation interaction constants. Here $B_e (\text{cm}^{-1}) = \hbar / 4\pi c \mu r_e^2$, where r_e is the equilibrium separation of the atoms and μ is the reduced mass.

The spin-orbit coupling constant has also been found to have a vibrational dependence by many researchers (11, 13, 14, 16). It is written as:

$$A_v = A_e - \chi_e (v + \frac{1}{2}) \quad . \quad (1.13)$$

When this is done, only a single $G(v)$ need be used to account for the vibrational energy of both components of the $^2\Pi$ ground state.



Lambda Doubling

It has already been pointed out that the eigenvalues of the symmetric and antisymmetric blocks in Table 1.2 are slightly different, each one giving the energy of one of the Λ -doublet levels. Herzberg (29) discusses this uncoupling phenomena in some detail. The splitting of the levels is symmetric and the energies, in this intermediate case are (5,9):

$$W_1^\Lambda(J, v) = T_1(J, v) \pm E_1^\Lambda(J, v) \quad (1.14)$$

Neglecting the term in $(E_{L-\Pi})^{-1}$, the effects of which are too small to be observed in this work, $E_1^\Lambda(v)$ is:

$$E_1^\Lambda(v) = 2p_\Lambda(J+\frac{1}{2}) + \left[\frac{4q_\Lambda}{\lambda_v-2} + \frac{2p_\Lambda}{(\lambda_v-2)^2} \right] [(J+\frac{1}{2})^3 - (J+\frac{1}{2})] \quad (1.15)$$

$$E_2^\Lambda = - \left[\frac{4q_\Lambda}{\lambda_v-2} + \frac{2p_\Lambda}{(\lambda_v-2)^2} \right] [(J+\frac{1}{2})^3 - (J+\frac{1}{2})] \quad (1.16)$$

Here p_Λ and q_Λ are the Λ -doubling constants.

Total Energy Expression

Finally to the order of approximation considered so far, the total energy of a diatomic molecule with a 2Π ground state and with a coupling scheme intermediate between Hund's cases (a) and (b) can be written:



$$\begin{aligned}
W_i^{\Lambda}(J, v) = & T_e + G(v) + B_v[(J+\frac{1}{2})^2 - \Lambda^2] + B_v[L(L+1) - \Lambda^2] \\
& + (-1)^i [L A_v(A_v - 4B_v)\Lambda^2 + B_v^2(J+\frac{1}{2})^2]^{\frac{1}{2}} \\
& - D_v[(J+\frac{1}{2})^4 - (J+\frac{1}{2})^2 + 1] \\
& + E_i^{\Lambda}(J, v)
\end{aligned} \tag{1.17}$$

where $i = 1(2)$ corresponds to the intermediate ${}^2\Pi_1$ (${}^2\Pi_3$) state respectively.

CHAPTER 2

WAVEFUNCTIONS AND INTENSITIES

The allowed transitions and intensities will now be considered. The expressions for the linear combinations of pure case (a) wave functions chosen as a basis for the energy calculations must be found.

Intermediate Wavefunctions

The linear combinations of symmetrized wavefunctions which diagonalize the 2×2 matrix of Eq. (1.7) are a good approximation for the system. For the intermediate wavefunctions one can write the matrix equation:

$$|{}^2\Pi\rangle^s, a = C |{}^2\Pi\rangle^s, a \quad , \quad (2.1)$$

where the wavefunctions $|{}^2\Pi\rangle$ and $|{}^2\Pi\rangle^s$ are in the intermediate and the symmetrized case (a) basis respectively. The s (a) denotes the symmetric (antisymmetric) linear combinations. The matrix C, is evaluated from $H^0 = CHC^\dagger$ and the normalization condition; $CC^\dagger = 1$. The result is:

$$C = \begin{pmatrix} a & -b \\ b & a \end{pmatrix} \quad , \quad (2.2)$$

where,

$$a_{Jv} = \left(\frac{X - 2 + \lambda}{2X} \right)^{\frac{1}{2}} \quad , \quad b_{Jv} = \left(\frac{X + 2 - \lambda}{2X} \right)^{\frac{1}{2}} \quad .$$



Therefore the intermediate wave functions to this order are:

$$|{}^2\Pi_{\frac{1}{2}}\rangle^{S,a} = a_{JV}|{}^2\Pi_{\frac{1}{2}}\rangle^{S,a} - b_{JV}|{}^2\Pi_{\frac{3}{2}}\rangle^{S,a} \quad (2.3a)$$

$$|{}^2\Pi_{\frac{3}{2}}\rangle^{S,a} = a_{JV}|{}^2\Pi_{\frac{3}{2}}\rangle^{S,a} + b_{JV}|{}^2\Pi_{\frac{1}{2}}\rangle^{S,a} \quad (2.3b)$$

The symmetries of the wave function have been carried merely as a formality since to the order considered here, the energies and therefore the wave functions are identical for both the symmetric and antisymmetric blocks of Table 1.2.

A complete tabulation of these wave functions for the states $v = 0$ and $v = 1$ and for J up to $49/2$ is given in Appendix II, for ${}^{14}\text{N}{}^{16}\text{O}$ and ${}^{15}\text{N}{}^{16}\text{O}$. It is seen that the wave functions are very nearly pure case (a).

Intensities

To obtain the selection rules and for later calculations, the integrated absorption coefficient (30, 31) (often called the absolute or integrated line intensity) S (cm^{-2}) will be needed. For a transition from the state m to m' it is:

$$S_{mm'} = (N_m - N_{m'}) h\nu_{mm'} B_{mm'} \quad , \quad (2.4)$$

where N_m is the number of absorbing molecules in the m^{th} state, $\nu_{mm'}$ is the frequency (cm^{-1}) of the transition, $B_{mm'}$ is the Einstein coefficient of induced absorption, and h is Planck's constant. For this work, $N_{m'}$ is negligible, and $B_{mm'}$ can be obtained from time-dependent perturbation theory (32). From this treatment it is seen that three cases must

Therefore the intermediate wave functions to this order are:

$$|^2\Pi_{\frac{1}{2}}\rangle^{S,a} = a_{JV} |^2\Pi_{\frac{1}{2}}\rangle^{S,a} - b_{JV} |^2\Pi_{\frac{3}{2}}\rangle^{S,a} \quad (2.3a)$$

$$|^2\Pi_{\frac{3}{2}}\rangle^{S,a} = a_{JV} |^2\Pi_{\frac{3}{2}}\rangle^{S,a} + b_{JV} |^2\Pi_{\frac{1}{2}}\rangle^{S,a} \quad (2.3b)$$

The symmetries of the wave function have been carried merely as a formality since to the order considered here, the energies and therefore the wave functions are identical for both the symmetric and antisymmetric blocks of Table 1.2.

A complete tabulation of these wave functions for the states $v = 0$ and $v = 1$ and for J up to $49/2$ is given in Appendix II, for $^{14}\text{N}^{16}\text{O}$ and $^{15}\text{N}^{16}\text{O}$. It is seen that the wave functions are very nearly pure case (a).

Intensities

To obtain the selection rules and for later calculations, the integrated absorption coefficient (30, 31) (often called the absolute or integrated line intensity) S (cm^{-2}) will be needed. For a transition from the state m to m' it is:

$$S_{mm'} = (N_m - N_{m'}) h\nu_{mm'} B_{mm'} \quad , \quad (2.4)$$

where N_m is the number of absorbing molecules in the m^{th} state, $\nu_{mm'}$ is the frequency (cm^{-1}) of the transition, $B_{mm'}$ is the Einstein coefficient of induced absorption, and h is Planck's constant. For this work, $N_{m'}$ is negligible, and $B_{mm'}$ can be obtained from time-dependent perturbation theory (32). From this treatment it is seen that three cases must

be considered. These are; a) no magnetic field, non-polarized radiation, b) longitudinal magnetic field, non-polarized radiation, and c) longitudinal magnetic field, radiation linearly polarized in the X-direction. (The values of B_{mm} , for these three cases are identical as they must be, but for completeness all are given here.) A coordinate system having the space fixed Z-axis parallel to an applied magnetic field and along the direction of propagation is chosen. (From this it is apparent that in later references to Zeeman patterns, it is a longitudinal effect that is being considered.)

In the following expressions $|\langle \mu_A \rangle|^2$ is the square of the absolute value of the space fixed electric dipole moment matrix element in the intermediate basis of the absorbing molecule, with $A = X, Y, Z$.

(a) No magnetic field, non-polarized radiation.

$$B_{mm} = \frac{2\pi}{3\hbar^2} \{ |\langle \mu_X \rangle|^2 + |\langle \mu_Y \rangle|^2 + |\langle \mu_Z \rangle|^2 \} \quad (2.5a)$$

This is effectively the case of isotropic radiation since the molecular dipole moments are randomly oriented. Since any direction is equivalent to any other, the three terms in the above sum may be replaced by 3 times any one of them.

(b) Longitudinal magnetic field, non-polarized radiation.

$$B_{mm} = \frac{2\pi}{2\hbar^2} \{ |\langle \mu_X \rangle|^2 + |\langle \mu_Y \rangle|^2 \} \quad (2.5b)$$

In writing this it has been assumed that the magnitude of the electric fields in the X- and Y-directions are equal.

- (c) Longitudinal magnetic field, radiation linearly polarized in the X-direction.

$$B_{mm'} = \frac{2\pi}{h^2} |(\mu_X)|^2 \quad (2.5c)$$

The electric dipole matrix elements must now be evaluated. For a diatomic molecule the body fixed dipole moment is along the internuclear or z-axis. The value of the A-component in the space fixed system is then:

$$\mu_A = \sum_{\alpha} \lambda_{A\alpha} \mu_{\alpha} = \lambda_{Az} \mu_z, \quad (2.6)$$

where $\lambda_{A\alpha}$ is the direction cosine transformation coefficient relating the A- (space fixed) and α -axis components of a vector, where $A = X, Y, Z$ and $\alpha = x, y, z$.

The quantum numbers v, J, Ω, M will describe the system completely for what is now needed. With primes denoting the final state the square of the absolute value of the matrix element of μ_A in the intermediate basis can be written (assuming no vibration-rotation interaction):

$$(\nu', J', \Omega', M_J' | \mu_A | \nu, J, \Omega, M_J)^2 = |(\nu' | \mu_z | \nu)|^2 |(\nu', J', \Omega', M_J' | \lambda_{Az} | \nu, J, \Omega, M_J)|^2. \quad (2.7)$$

The term, $|(\nu' | \mu_z | \nu)|^2$ is a vibration transition probability and will be designated $|R_v|^2$. The non-zero elements for this quantity, assuming anharmonic oscillator wavefunctions,

will occur (33) for $v' = v \pm 1, \pm 2, \pm 3 \dots$. Cross, Hainer and King (34) have shown that the second matrix element of Eq. (2.7) can be written:

$$(J', \Omega', M_J' | \lambda_{AZ} | J, \Omega, M_J) = \phi_{AZ}(J'; J) \phi_{AZ}(J', \Omega'; J, \Omega) \phi_{AZ}(J', M'; J, M) \quad (2.8)$$

Table 2.1 lists the values for these terms as they apply to the pure case (a) representation. It is noted that only the term $\phi_{AZ}(J', \Omega'; J, \Omega)$ will be affected by the intermediate wavefunctions. It is also true that $|(\mu_X)|^2 = |(\mu_Y)|^2$ so that the only element which need be calculated is $|(\mu_X)|^2$.

The pure case (a) angular momentum selection rules for this coordinate system may be seen directly from these matrix elements. They are $\Delta J = -1, 0, +1$ corresponding to the P, Q, and R branches respectively, $\Delta \Omega = 0$ which implies $\Delta \Sigma = 0$ (since we are considering transitions within the $^2\Pi$ state $\Delta \Lambda = 0$) and $\Delta M = \pm 1$.

Since only the ϕ_{AZ} components will need to be considered, the subscript will be dropped. The absolute square of the non-zero terms in Eq. (2.8) are as follows:

$$(i) \quad |\phi(J-1; J)|^2 = [16J^2(2J+1)(2J-1)]^{-1} \quad (2.9a)$$

$$|\phi(J; J)|^2 = [16J^2(J+1)^2]^{-1} \quad (2.9b)$$

$$|\phi(J+1; J)|^2 = [16(J+1)^2(2J+1)(2J+3)]^{-1} \quad (2.9c)$$



Table 2.1 Direction Cosine Matrix Elements (34).

	$J' = J+1$	$J' = J$	$J' = J-1$
$\phi_{A\alpha}(J'; J)$	$\{4(J+1)[(2J+1)(2J+3)]^{\frac{1}{2}}\}^{-1}$	$[4J(J+1)]^{-1}$	$\{4[(2J+1)(2J-1)]^{\frac{1}{2}}\}^{-1}$
$\phi_{Az}(J', \Omega; J, \Omega)$	$2[(J+\Omega+1)(J-\Omega+1)]^{\frac{1}{2}}$	2Ω	$-2[J^2-\Omega^2]^{\frac{1}{2}}$
$\phi_{Ay}(J', \Omega^{\pm 1}; J, \Omega)$	$\mp [(J^{\pm}\Omega+1)(J^{\pm}\Omega+2)]^{\frac{1}{2}}$	$[(J^{\pm}\Omega)(J^{\pm}\Omega+1)]^{\frac{1}{2}}$	$\mp [(J^{\pm}\Omega)(J^{\pm}\Omega-1)]^{\frac{1}{2}}$
$= \mp i \phi_{Ax}(J', \Omega^{\pm 1}; J, \Omega)$			
$\phi_{Z\alpha}(J', M; J, M)$	$2[(J+M+1)(J-M+1)]^{\frac{1}{2}}$	$2M$	$-2[J^2-M^2]^{\frac{1}{2}}$
$\phi_{Y\alpha}(J', M^{\pm 1}; J, M)$	$\mp [(J^{\pm}M+1)(J^{\pm}M+2)]^{\frac{1}{2}}$	$[(J^{\pm}M)(J^{\pm}M+1)]^{\frac{1}{2}}$	$\mp [(J^{\pm}M)(J^{\pm}M-1)]^{\frac{1}{2}}$
$= \mp i \phi_{X\alpha}(J', M^{\pm 1}; J, M)$			



(ii) Here the notation Ω_1, Ω_2 for $\Omega = \frac{1}{2}, \frac{3}{2}$ respectively is used.

(a) $\Delta\Omega = 0$

$$|\Phi(J-1, \Omega_{1,2}; J, \Omega_{1,2})|^2 = 4\{a_{J-1,v} a_{J,v} [J^2 - \Omega_{1,2}^2]^{\frac{1}{2}} + b_{J-1,v} b_{J,v} [J^2 - \Omega_{2,1}^2]^{\frac{1}{2}}\}^2 \quad (2.10a)$$

$$|\Phi(J, \Omega_{1,2}; J, \Omega_{1,2})|^2 = 4\{a_{J,v} a_{J,v} \Omega_{1,2} + b_{J,v} b_{J,v} \Omega_{2,1}\}^2 \quad (2.10b)$$

$$|\Phi(J+1, \Omega_{1,2}; J, \Omega_{1,2})|^2 = 4\{a_{J+1,v} a_{J,v} [(J+1)^2 - \Omega_{1,2}^2]^{\frac{1}{2}} + b_{J+1,v} b_{J,v} [(J+1)^2 - \Omega_{2,1}^2]^{\frac{1}{2}}\}^2 \quad (2.10c)$$

(b) $\Delta\Omega = \pm 1$

$$|\Phi(J-1, \Omega_{2,1}; J, \Omega_{1,2})|^2 = 4\{a_{J-1,v} b_{J,v} [J^2 - \Omega_{2,1}^2]^{\frac{1}{2}} - b_{J-1,v} a_{J,v} [J^2 - \Omega_{1,2}^2]^{\frac{1}{2}}\}^2 \quad (2.11a)$$

$$|\Phi(J, \Omega_{2,1}; J, \Omega_{1,2})|^2 = 4\{a_{J,v} b_{J,v} \Omega_{2,1} - b_{J,v} a_{J,v} \Omega_{1,2}\}^2 \quad (2.11b)$$

$$|\Phi(J+1, \Omega_{2,1}; J, \Omega_{1,2})|^2 = 4\{a_{J+1,v} b_{J,v} [(J+1)^2 - \Omega_{2,1}^2]^{\frac{1}{2}} - b_{J+1,v} a_{J,v} [(J+1)^2 - \Omega_{1,2}^2]^{\frac{1}{2}}\}^2 \quad (2.11c)$$

It is to be noted that in the intermediate basis the values $\Delta\Omega = \pm 1$ are allowed, for here the quantum number Ω merely denotes the limiting pure case (a) value. The

following terms give the relative intensities of the Zeeman components for each branch:

$$(iii) \quad |\Phi(J+1, M \pm 1; J, M)|^2 = (J+M)(J+M-1) \quad (2.12a)$$

$$|\Phi(J, M \pm 1; J, M)|^2 = (J+M)(J+M+1) \quad (2.12b)$$

$$|\Phi(J+1, M \pm 1; J, M)|^2 = (J+M+1)(J+M+2) \quad (2.12c)$$

The line strength for a particular branch is obtained from the product of the appropriate ΔJ terms from Eqs. (2.9) and (2.10) or (2.11) multiplied by the sum over all possible M and ΔM values of the corresponding term from Eq. (2.12).

These sums are:

$$\sum_M [(J-M)(J-M-1) + (J+M)(J+M-1)] = \frac{4}{3}J(2J+1)(2J-1) \quad (2.13a)$$

$$\sum_M [(J+M)(J+M+1) + (J-M)(J-M+1)] = \frac{4}{3}J(J+1)(2J+1) \quad (2.13b)$$

$$\sum_M [(J+M+1)(J+M+2) + (J-M+1)(J-M+2)] = \frac{4}{3}(J+1)(2J+1)(2J+3) \quad (2.13c)$$

Then defining $s(J', \Omega'; J, \Omega)$ as the line strength, one can write:

$$s(J-1, \Omega'; J, \Omega) = \frac{1}{12J} |\Phi(J-1, \Omega'; J, \Omega)|^2 \quad (2.14a)$$

$$s(J, \Omega'; J, \Omega) = \frac{(2J+1)}{12J(J+1)} |\Phi(J, \Omega'; J, \Omega)|^2 \quad (2.14b)$$

$$s(J+1, \Omega'; J, \Omega) = \frac{1}{12(J+1)} |\Phi(J+1, \Omega'; J, \Omega)|^2 \quad (2.14c)$$



The calculated values for these line strengths are given in Appendix III for the four possible bands (i.e., $\Delta\Omega$ transitions) up to $J = 49/2$ for $^{14}\text{N}^{16}\text{O}$ and $^{15}\text{N}^{16}\text{O}$. The values of the line strength for the $\Delta\Omega = \pm 1$ transitions are seen to be considerably less than those for $\Delta\Omega = 0$.

The effect of the symmetry of the wave functions has been neglected here. It has been shown that for each value of J there are two levels (Λ -doublet levels) of opposite parity. The general symmetry selection rule is (35):

$$+ \leftrightarrow -, + \nleftrightarrow +, - \nleftrightarrow - . \quad (2.15)$$

Each line of a branch will consist of two transitions of equal intensity, and the line strengths given above must be divided by 2 to properly account for this Λ -doubling.

The Einstein coefficient of induced absorption may now be given. For the field free case it is:

$$B(v', J', \Omega'; v, J, \Omega) = \frac{2\pi}{h^2} |R_v|^2 S(J', \Omega'; J, \Omega) . \quad (2.16)$$

In the presence of a magnetic field, the values given in the preceding equation must be multiplied by a field factor corresponding to the particular branch needed. This gives:

$$B(v', J-1, \Omega', M \pm 1; v, J, \Omega, M) =$$

$$B(v', J-1, \Omega'; v, J, \Omega) \left(\frac{3}{4J} \frac{(J+M)(J+M-1)}{(2J+1)(2J-1)} \right) \quad (2.17a)$$

$$B(v', J, \Omega', M \pm 1; v, J, \Omega, M) =$$

$$B(v', J, \Omega'; v, J, \Omega) \left[\frac{3}{4} \frac{(J \mp M)(J \pm M + 1)}{J(J+1)(2J+1)} \right] \quad (2.17b)$$

$$B(v', J+1, \Omega', M \pm 1; v, J, \Omega, M) =$$

$$B(v', J+1, \Omega'; v, J, \Omega) \left[\frac{3}{4} \frac{(J \pm M + 1)(J \pm M + 2)}{(J+1)(2J+1)(2J+3)} \right]. \quad (2.17c)$$

Here again the symmetry of the levels has been neglected.

Finally an expression for the number of absorbing molecules in the initial state is needed. This can be obtained from Boltzmann statistics. If N is the total number of absorbers taking part in the absorption process/unit volume, then the number of absorbers in the state characterized by the numbers i, v, J, M (i denoting the electronic state) will be given to a very good approximation by:

$$N_{ivJM} = N \exp(-\epsilon_i/kT) \exp(-\omega_e v/kT) \times \\ \exp[-B_v J(J+1)/kT] \exp(-\Delta/kT) / Z_i Z_v Z_J Z_M \quad (2.18)$$

where B_v is the rotational constant, Δ is the Zeeman energy of the state M , and Z_i, Z_v, Z_J and Z_M are partition functions for the electronic, vibrational, rotational and magnetic states. Since the magnetic energies are small compared with kT the magnetic term becomes:

$$\frac{\exp(-\Delta/kT)}{Z_M} \approx \frac{1}{(2J+1)} \quad (2.19)$$

The evaluation of the vibrational and rotational terms is given in many places (see e.g. Townes and Schawlow (36)).

They can be written:

$$\frac{\exp(-\omega_e v/kT)}{Z_v} = \exp(-\omega_e v/kT) [1 - \exp(-\omega_e/kT)] \quad (2.20)$$

and

$$\frac{\exp[-B_v J(J+1)/kT]}{Z_J} \approx \frac{(2J+1)B_v}{kT} \exp[-B_v J(J+1)/kT] \quad (2.21)$$

For the case of nitric oxide only the 2Π electronic states need be considered in evaluating the electronic term. This becomes:

$$\frac{\exp(-\epsilon_{1,2}/kT)}{Z_i} = \frac{1}{1 + \exp(\mp \Delta\epsilon/kT)} \quad (2.22)$$

where $\Delta\epsilon = E_2 - E_1 = A$ (the spin-orbit constant). It must be remembered that the $-(+)$ sign above is used for the transition $\Omega = \frac{1}{2}$, $\Delta\Omega = 0, +1$ ($\Omega = \frac{3}{2}$, $\Delta\Omega = 0, -1$).

The complete expression for the integrated absorption coefficient in the absence of a magnetic field is then obtained from the product of Eqs. (2.16), (2.19), (2.20), (2.21), and (2.22) as:

$$S(v', J', \Omega'; v, J, \Omega) =$$

$$\frac{2\pi^2 B_v P}{(kT)^2} \frac{\exp(-\omega_e v/kT) [1 - \exp(-\omega_e/kT)]}{[1 + \exp(\mp \Delta\epsilon/kT)]} \times$$

$$\exp[-B_v J(J+1)/kT] B(v', J', \Omega'; v, J, \Omega) v(v', J', \Omega'; v, J, \Omega) \quad (2.23)$$

where P is the partial pressure of the absorbing gas (the ideal gas law has been used) and all other quantities are

as previously defined.

The integrated absorption coefficient is usually written in the form:

$$S = S_0 P \quad (2.24)$$

where S_0 is given in $\text{cm}^{-2}/\text{atm}$.

By making use of James' (12) experimental determination of $|R_v|^2 = (8.14 \times 10^{-2} \text{ Debye})^2$ the values of S_0 can be calculated. This was done for $^{14}\text{N}^{16}\text{O}$ for the vibrational transition $v=0 \rightarrow v=1$ for values of J up to $49/2$ for all possible values of $\Delta\Omega$ and ΔJ . These are tabulated in Appendix IV. Shaw and Abels (38) have also carried out portions of this calculation though by a different method.

Transitions

The pure case (a) selection rules, the intermediate wavefunctions, the intensities and the energies having already been given, the spectrum can be predicted. The main points should be summarized. It will consist of two subbands, ${}^2\Pi_{1/2} \rightarrow {}^2\Pi_{1/2}$ and ${}^2\Pi_{3/2} \rightarrow {}^2\Pi_{3/2}$ and two satellite bands, ${}^2\Pi_{1/2} \rightarrow {}^2\Pi_{3/2}$ and ${}^2\Pi_{3/2} \rightarrow {}^2\Pi_{1/2}$ for the particular vibration being considered. To facilitate later notation these transitions will be designated 1, 2, H, and L respectively. The two satellite transitions may also be called HES and LES (high and low energy satellite) respectively. Each of these transitions will have a P, Q and R branch corresponding to $\Delta J = -1, 0, +1$ respectively. In addition each

line of these branches will be a doublet, since for each value of J , there are two levels of opposite parity. A typical spectral line within a vibration-rotation band might be labeled $\text{PH}(7/2)+$, which indicates a transition from $J = 7/2, \Omega = \frac{1}{2}$ to $J = 5/2, \Omega = \frac{3}{2}$. The plus sign is merely a designation to indicate the higher frequency component of the Λ -doublet.



CHAPTER 3

ZEEMAN ENERGIES

The intensities and selection rules for the Zeeman transitions were given in the preceding chapter. Here our concern will be the energy levels of the system in the presence of a magnetic field. The effect of the intermediate wavefunctions will be quite apparent, for contrary to the pure case (a) coupling scheme where the $^2\Pi_{1/2}$ state would have a magnetic moment of zero, a non-zero value is now obtained. Dousmanis, Sanders and Townes (20) have given a treatment of the Zeeman energies in the intermediate case.

The magnetic Hamiltonian is:

$$H_m = - \vec{\mu} \cdot \vec{H} \quad . \quad (3.1)$$

In the body fixed system the magnetic moment operator is:

$$\vec{\mu} = -\mu_0 (\vec{L} + 2\vec{S}) \quad (3.2)$$

where μ_0 is the Bohr magneton.

Since this work is concerned with only the $^2\Pi$ states, only the z-component of L will have non-zero matrix elements. To transform the magnetic moment operator to the space fixed system the direction cosines, $\lambda_{A\alpha}$, must again be used. Since the magnetic field is taken along the space fixed Z-axis, only this component of the magnetic moment is needed, viz.



$$\mu_Z = -\mu_0 [2\lambda_{zx} S_x + 2\lambda_{zy} S_y + \lambda_{zz} (\Lambda + 2S_z)] \quad (3.3)$$

From Appendix I and Table 2.1 the matrix elements of μ_Z can be calculated by a simple direct product of $\lambda_{\alpha\alpha}$ and S_{α} .

In the pure case (a) basis the matrix elements needed are:

$$\langle J, \Omega, M | \mu_Z | J, \Omega, M \rangle = \frac{-\mu_0 \Omega M}{J(J+1)} (\Lambda + 2\Sigma) \quad (3.4a)$$

$$\begin{aligned} \langle J, \Omega \pm 1, M | \mu_Z | J, \Omega, M \rangle &= \frac{+\mu_0 [(J \mp \Omega) (J \pm \Omega + 1)]^{\frac{1}{2}} M}{J(J+1)} \times \\ & [S(S+1) - \Sigma(\Sigma \pm 1)]^{\frac{1}{2}} \quad (3.4b) \end{aligned}$$

Inserting the appropriate values for the quantum numbers yields:

$$\langle {}^2\Pi_{\frac{1}{2}} | \mu_Z | {}^2\Pi_{\frac{1}{2}} \rangle = 0 \quad (3.5a)$$

$$\langle {}^2\Pi_{\frac{3}{2}} | \mu_Z | {}^2\Pi_{\frac{3}{2}} \rangle = \frac{-3\mu_0 M}{J(J+1)} \quad (3.5b)$$

$$\langle {}^2\Pi_{\frac{1}{2}} | \mu_Z | {}^2\Pi_{\frac{3}{2}} \rangle = \langle {}^2\Pi_{\frac{3}{2}} | \mu_Z | {}^2\Pi_{\frac{1}{2}} \rangle = \frac{+\mu_0 M}{J(J+1)} [(J - \frac{1}{2}) (J + \frac{3}{2})]^{\frac{1}{2}} \quad (3.5c)$$

From this the expectation values for μ_Z in the intermediate basis can be calculated, viz.

$$(\mu_Z) = \frac{-\mu_0 M}{J(J+1)} \left\{ \frac{3}{2} \pm \frac{[2(J - \frac{1}{2})(J + \frac{3}{2}) + 3 - \frac{3}{2}\lambda]}{X} \right\} \quad (3.6)$$

where the upper (lower) sign corresponds to the intermediate ${}^2\Pi_{\frac{1}{2}}$ (${}^2\Pi_{\frac{3}{2}}$) state.



The Zeeman energies can be written:

$$E_{JM} = g_J \mu_0 M H \quad , \quad (3.7)$$

where g_J is the molecular g -factor given by dividing Eq. (3.6) by $-\mu_0 M$. Calculated values for g_J are given in Appendix V for the vibrational states $v = 0$ and $v = 1$ and for J -values through $49/2$ for both $^{14}\text{N}^{16}\text{O}$ and $^{15}\text{N}^{16}\text{O}$.

Eq. (3.6) agrees with that given by DST (20) although the method by which it was obtained follows that of Lin (39).

The strengths obtained for the Zeeman components in Chap. 2 did not include the perturbing effect of the magnetic field. They are certainly good to a first approximation and will be used throughout.

If one were to consider $H_m = -\vec{\mu} \cdot \vec{H}$, as a perturbation, the perturbed intermediate rotational wave functions, from first order perturbation theory (40), can be written:

$$|J, \Omega, M\rangle^1 = |J, \Omega, M\rangle + \frac{(J+1, \Omega, M | \mu_Z | J, \Omega, M) H}{\Delta E_R} |J+1, \Omega, M\rangle \\ - \frac{(J-1, \Omega, M | \mu_Z | J, \Omega, M) H}{\Delta E_P} |J-1, \Omega, M\rangle \quad , \quad (3.8)$$

where $\Delta E_{R,P} = E_{J+1} - E_J$ and $E_J - E_{J-1}$ respectively. This approach was carried out for a pure case (a) basis and the results indicated that the intensities would change by less than 1%. The exact perturbation calculation is not conceptually difficult; however, the algebra involved, because of two magnetically sensitive levels, will be extremely tedious.



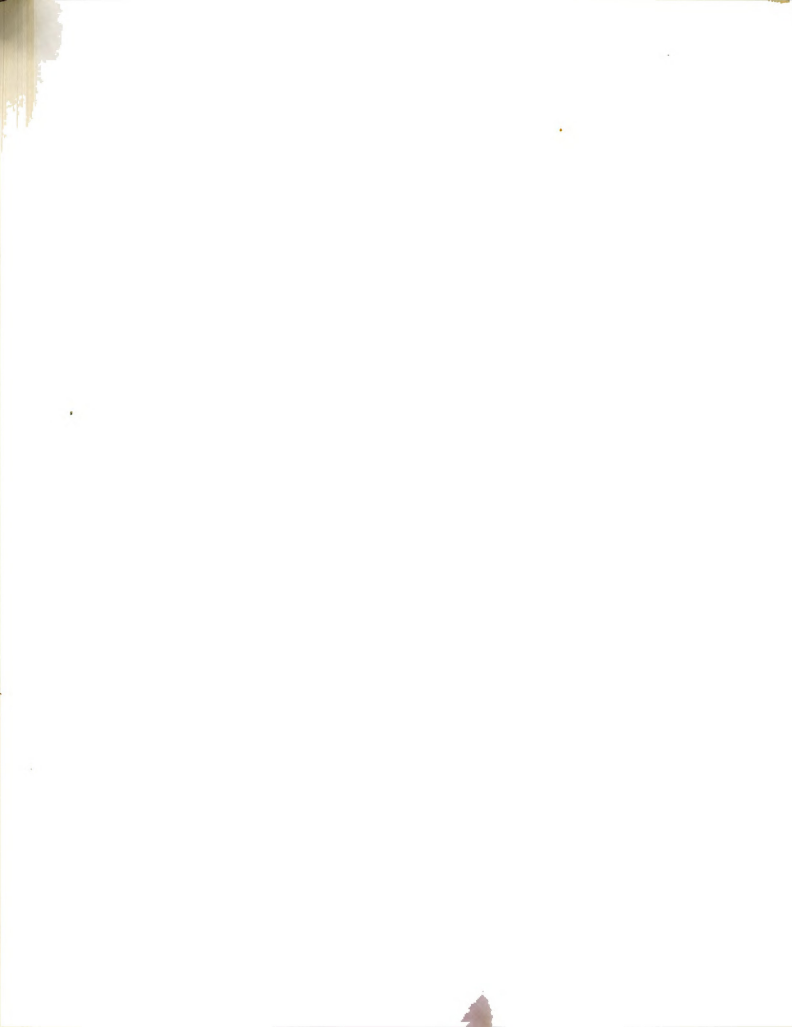
CHAPTER 4

MAGNETIC ROTATION THEORY

As early as 1846 Faraday (41) showed that optical activity (rotation of the plane of polarization) can be induced in matter by a magnetic field. This furnished one of the first connections between optics and magnetism and provided an impressively strong hint as to the electromagnetic character of light.

A medium exhibits magnetic circular birefringence (MCB) (or Faraday rotation) when, as the name implies, a longitudinal magnetic field causes the refractive indices for right and left circularly polarized light to be unequal, thereby rotating the plane of polarization. In addition the field causes different absorption coefficients for the two polarizations, giving rise to magnetic circular dichroism (MCD). These two effects are interrelated. Magnetic rotation spectra (MRS) in which the total intensity transmitted through crossed polarizers is measured, stems from these two effects.

Buckingham and Stephens (B&S) (21) have recently given an extensive review of magnetic optical activity from a phenomenological standpoint. Their starting point is essentially that of Rosenfeld (42), Kramers (43) and Serber (44) with



the extensions of Carroll (45). It should be mentioned that Hameka (46, 47, 48) has treated magneto-optic phenomena by resonance fluorescence techniques. While this is probably a more rigorous approach, it loses sight of the relevant phenomenological parameters and consequently will not be considered here.

The phenomenological calculation considered by B&S is carried out in three steps: the observable is related to the difference in the complex refractive indices of right and left circularly polarized light; Maxwell's equations are used to express the complex indices in terms of the moments induced by the radiation; finally, these moments are calculated quantum mechanically.

This approach is general enough to be applicable to all material phases; however, things can be simplified, both conceptually and practically, for the gaseous phase which is our immediate concern.

The approach which will be used is an extension of that of Aubel (22), and parallels quite closely that of B&S. The first step of both approaches is the same.

In complex notation the electric vector describing a circularly polarized wave propagating in the +Z-direction is (21):

$$E^{\pm} = E_x \hat{i} \pm i E_y \hat{j} = E_0 \exp[i(\omega t - k^{\pm} Z)] (\hat{i} \pm i \hat{j}) \quad (4.1)$$

where E^+ (E^-) represents the electric field for a right (left) circular polarization in the conventional right hand

sense (i.e., for radiation traveling in the +Z-direction, right circularly polarized will mean a rotation of the electric vector in the counter-clockwise sense viewed into the beam), k^+ (k^-) is the corresponding propagation constant, and ω is the angular frequency of the radiation.

Then a wave linearly polarized in the X- and Y-directions can be written in terms of E^+ and E^- :

$$E_X = \frac{1}{2}(E^+ + E^-) \quad (4.2a)$$

$$E_Y = \frac{1}{2i}(E^+ - E^-) \quad (4.2b)$$

For an optically active media there will be two different indices of refraction:

$$n^\pm = \frac{ck^\pm}{\omega} \quad (4.3)$$

If a wave initially linearly polarized in the X-direction traverses an absorbing media of length L, then upon emerging there will be a Y-component given by:

$$E_Y = \frac{E_0}{2i} \{ \sqrt{T^+} \exp[i(\omega t + P - \frac{n^+ \omega L}{c})] - \sqrt{T^-} \exp[i(\omega t - P - \frac{n^- \omega L}{c})] \} \quad (4.4)$$

T^+ and T^- are the transmission fractions for the right and left circularly polarized components respectively. The ratio of the intensity transmitted by an analyzer whose axis is parallel to the Y-direction relative to that of one at an angle P relative to the X-direction and in the absence of the media is:



$$\begin{aligned}
T' &\equiv \frac{|E_Y|^2}{|E_0|^2} = \frac{1}{4} \left\{ T^+ + T^- - \sqrt{T^+ T^-} \exp\{i[2P + \frac{\omega L}{c}(n^- - n^+)]\} \right. \\
&\quad \left. - \sqrt{T^+ T^-} \exp\{-i[2P + \frac{\omega L}{c}(n^- - n^+)]\} \right\} \\
&= \frac{1}{4} \{ T^+ + T^- - 2\sqrt{T^+ T^-} \cos 2(P + \theta) \} \quad , \quad (4.5)
\end{aligned}$$

where $\theta = \pi \nu L (n^- - n^+)$ and ν is the frequency in cm^{-1} .

Assuming a normal exponential law of absorption, the transmission fraction is given:

$$T^\pm = \exp(-\alpha^\pm L) \quad , \quad (4.6)$$

where α^+ (α^-) is the absorption coefficient for right (left) circularly polarized light. One usually defines a quantity:

$$\phi \equiv \frac{L}{2} (\alpha^- - \alpha^+) \quad . \quad (4.7)$$

With this, Eq. (4.5) can be written:

$$T' = \left\{ \left(\frac{\sqrt{T^+} - \sqrt{T^-}}{2} \right)^2 + \sqrt{T^+ T^-} \sin^2(P + \theta) \right\} \quad (4.8a)$$

$$= \exp\left[-\frac{(\alpha^+ + \alpha^-)L}{2}\right] \{ \sin^2(P + \theta) + \sinh^2 \phi \} \quad . \quad (4.8b)$$

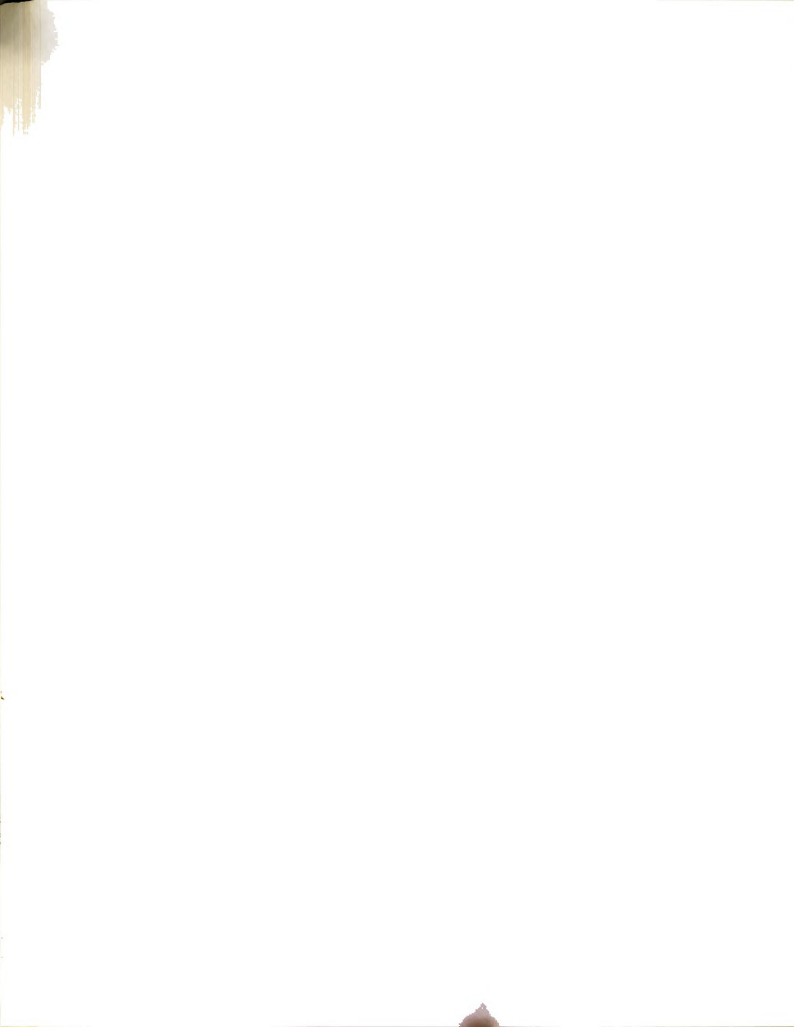
It should be understood that $n^\pm$, $\alpha^\pm$ and therefore θ , ϕ and T' are functions of frequency. The form of Eq. (4.8a) makes it easy to separate it into a circular dichroism term:

$$CD = \frac{[\sqrt{T^+} - \sqrt{T^-}]^2}{4} = \frac{\{\exp(-\frac{\alpha^+ L}{2}) - \exp(-\frac{\alpha^- L}{2})\}^2}{4} \quad (4.9a)$$

and a circular birefringence term:

$$CB = \sqrt{T^+ T^-} \sin^2(P + \theta) = \exp\left[-\frac{(\alpha^+ + \alpha^-)L}{2}\right] \sin^2(P + \theta) \quad . \quad (4.9b)$$

This completes step one.



At step two B&S obtain the complex indices in terms of the magnetic and electric polarizabilities. Following Aubel it is simpler to express them in terms of the absorption coefficients for right and left circularly polarized light. From Penner (49) one finds that the absorption coefficient can be written in the following forms for various conditions of pressure.

At very low pressure, Doppler broadening is the major contribution to line width. The absorption coefficient is:

$$\alpha_D(\nu_i) = \frac{S}{\gamma_D} \left(\frac{\ln 2}{\pi} \right)^{1/2} \exp \left[\frac{-\ln 2}{\gamma_D} (\nu - \nu_i)^2 \right] \quad (4.10)$$

where S is the integrated absorption coefficient, γ_D is the Doppler halfwidth, and ν_i is the frequency of the i^{th} absorption line. In speaking of halfwidths, it will always be assumed to mean one half the total width at one half the maximum height (HWHM) unless otherwise designated. The Doppler halfwidth is given by:

$$\gamma_D = \frac{\nu_i}{c} \left[\frac{2kT}{M} \ln 2 \right]^{1/2} \quad (4.11)$$

where k is the Boltzmann constant, M the mass of the molecule and T the absolute temperature.

At the other extreme, that of high pressure, the line shape should be Lorentzian and the absorption coefficient will be:

$$\alpha_L(\nu_i) = \frac{S\gamma_L}{\pi} \frac{1}{(\nu - \nu_i)^2 + \gamma_L^2} \quad (4.12)$$

where γ_L is the Lorentz halfwidth and S is as before.



γ_L is pressure dependent and can be written (50):

$$\gamma_L = \gamma_L^0 P, \quad (4.13)$$

where P is the pressure. Values for γ_L^0 ($\text{cm}^{-1}/\text{torr}$) must be found experimentally.

Most of our work falls in an intermediate pressure range where the absorption coefficient is:

$$\alpha(\nu_i) = \frac{S\gamma_L}{\gamma_D} \left(\frac{\ln 2}{\pi^3} \right)^{\frac{1}{2}} \int_{-\infty}^{\infty} \frac{\exp[-(\ln 2 / \gamma_D^2) \eta^2] d\eta}{\gamma_L^2 + (\nu - \nu_i - \eta)^2}. \quad (4.14)$$

If there is an applied longitudinal magnetic field there will be an absorption coefficient for each Zeeman component. When the absorption coefficient for each ν_i has been found, the total absorption coefficient is found for right or left circular polarizations by a single summation:

$$\alpha^{\pm}(\nu) = \sum_i \alpha^{\pm}(\nu_i). \quad (4.15)$$

The integrated absorption coefficient determines whether ν_i absorbs the right or left component as will be shown shortly.

Finally the Kramers-Kronig relations (51) are used to obtain the indices of refraction, viz.

$$\theta(\nu) = \frac{1}{\pi} \int_0^{\infty} \frac{\nu' \phi(\nu') d\nu'}{(\nu'^2 - \nu^2)} \quad (4.16a)$$

$$\phi(\nu) = -\frac{\nu}{\pi} \int_0^{\infty} \frac{\theta(\nu') d\nu'}{(\nu'^2 - \nu^2)} \quad (4.16b)$$



The quantum mechanical calculation of the integrated absorption coefficient which was treated in Chapter 2, completes the third step. From time dependent perturbation theory it is known (52) that $\Delta M = +1$ (-1) absorbs right (left) circularly polarized radiation.

This completes the phenomenological calculation and one must now combine Eqs. (4.6), (4.7), (4.8a), (4.14), (4.15) and (4.16a) to obtain, in principle, the magnetic rotation intensity $T'(\nu)$ as would be observed by a spectrometer having infinite resolving power.

In practice the spectrometer halfwidth is much greater than the line widths being considered. Therefore to predict the MRS signal which would be observed, an integration over the spectrometer slit-function must be performed. The normalized MRS signal will then be given by:

$$T(\nu) = \frac{\int T'(\nu) \sigma(\nu) d\nu}{\int \sigma(\nu) d\nu} . \quad (4.17)$$

Here $\sigma(\nu)$ is the spectrometer slit-function which can be obtained by recording the profile of a very narrow emission line.

It should be mentioned that the integrations involved in Eqs. (4.14), (4.16) and (4.17) can not be done in closed form and numerical integration techniques must be used.

CHAPTER 5

ABSORPTION ANALYSIS

Spectra of the 1- and 2-subbands, the HES and LES for the $v = 0 \rightarrow v = 1$ transition for both $^{14}\text{N}^{16}\text{O}$ and $^{15}\text{N}^{16}\text{O}$ were obtained using the high resolution infrared spectrometer. Details of the instrument will be treated in Chapter 8. Experimental details for obtaining the absorption spectra of the four bands of both $^{14}\text{N}^{16}\text{O}$ and $^{15}\text{N}^{16}\text{O}$ are given in Table 5.1. Figures 5.1 and 5.2 show typical absorption records for portions of the HES and LES spectra for $^{15}\text{N}^{16}\text{O}$. $^{15}\text{N}^{16}\text{O}$ and $^{14}\text{N}^{16}\text{O}$ were obtained from the Isomet Corporation and the Matheson Company respectively. $^{15}\text{N}^{16}\text{O}$ had sufficient purity as obtained; however, the $^{14}\text{N}^{16}\text{O}$ contained nitrogen compound impurities which were frozen out for the LES region.

Calibration was accomplished using Edser-Butler bands as recently reviewed (53). Bands of CO, HCl, and HCN measured by Rank et. al. (53) were used as standards. Standard deviations of the calibration fits ranged from 0.001 cm^{-1} to 0.003 cm^{-1} . All frequencies used in the analysis were measured on at least two different records.

The absorption charts were photographed, the raw data then digitized using the Hydel system (54) and finally reduced to absorption frequencies by the computer program SHAFT, which

Table 5.1 Experimental Conditions for Absorption Spectra.

$^{14}\text{N}^{16}\text{O}$						Calibration			
Chart	Band	Region (cm^{-1})	Pressure (Torr)	Fringe Order	Eff. Sl. Width (cm^{-1})	Standard	Order	Pressure (Torr)	S.D.
5/26	HES	1945-2070	100-200	9	.062	HCl (2-0)	3	10-20	0.0014
5/27	HES	1990-2020	200	9	.062	CO (1-0)	1	1	
5/31-1	HES	1990-2020	200	9	.062	CO (1-0)	1	80-3	0.0015
5/31-2	HES	1990-2020	200	9	.062	CO (1-0)	1	80-3	0.0012
5/31-3	HES	1990-2020	100	9	.062	CO (1-0)	1	80-3	0.0010
6/1-1	HES	1990-2020	100	9	.062	CO (1-0)	1	80-3	0.0015
6/1-2	HES	1990-2020	100	9	.062	CO (1-0)	1	77-9	0.0017
6/1-2	HES	1995-2080	100-200	9	.062	CO (1-0)	1	80-1	0.0021
6/2-1	HES	1995-2080	100-200	9	.062	CO (1-0)	1	80-1	0.0023
6/2-2	HES	1950-1990	100-200	9	.062	HCl (2-0)	3	6-10	0.0015
6/3	HES	1950-1990	100-200	9	.062	CO (1-0)	1	50-10	
6/7	FUND	1905-1990	1-260	9	.062	HCl (2-0)	3	6-14	0.0012
6/10	FUND	1905-1990	1-260	9	.062	CO (1-0)	1	50-10	
6/13	FUND	1800-1930	.5-2	9	.061	HCl (2-0)	3	4	0.0013
6/14	FUND	1800-1910	.5-2	9	.061	CO (1-0)	1	50-10	
6/22	FUND	1705-1800	230-2	11	.059	HCl (2-0)	3	4	0.0016
6/23	FUND	1705-1800	200-2	10	.059	CO (1-0)	1	50-8	
6/24	LES	1670-1830	250-100	10	.062	HCN (101)	3	5	0.0020
7/5	LES	1670-1840	200-100	11	.062	HCl (2-0)	3	6-9	
11/1	LES	1690-1795	100	10	.036	HCN (101)	3	5	0.0022
11/2	LES	1690-1795	100	11	.036	HCl (2-0)	3	6-10	
7/11	HES	1930-2020	76	9	.060	HCN (001)	2	4-10	0.0022
7/13	HES	1920-2015	75	9	.060	HCN (101)	3	5	
7/15	LES	1690-1780	71	10	.062	HCN (001)	2	5-10	0.0013
7/18-1	LES	1660-1690	70	10	.055	HCN (101)	3	5	
7/18-2	LES	1645-1690	70	11	.055	HCN (001)	2	1	0.0019
7/19	LES	1700-1780	68	11	.062	HCl (2-0)	3	10-6	
7/20	FUND	1705-1790	66-2	10	.065	HCN (001)	2	1-2	0.0019
7/21-1	FUND	1710-1790	66-2	11	.065	HCl (2-0)	3	9-6	
7/21-2	FUND	1770-1890	.5-2	9	.057	HCN (001)	2	2	0.0030
7/22	FUND	1790-1890	.5-2	9	.057	HCN (101)	3	5-3	
7/25	FUND	1890-1970	1-64	9	.058	HCN (001)	2	2	0.0038
7/26	FUND	1890-1970	1-64	9	.058	HCN (101)	3	3	
7/11	HES	1930-2020	76	9	.060	HCl (2-0)	3	4-3	0.0016
7/13	HES	1920-2015	75	9	.060	CO (1-0)	1	3-1	
7/15	LES	1690-1780	71	10	.062	HCl (2-0)	3	4-3	0.0018
7/18-1	LES	1660-1690	70	10	.055	CO (1-0)	1	3-2	
7/18-2	LES	1645-1690	70	11	.055	HCN (001)	2	1-2	0.0020
7/19	LES	1700-1780	68	11	.062	HCN (101)	3	4	
7/20	FUND	1705-1790	66-2	10	.065	HCN (001)	2	1	0.0021
7/21-1	FUND	1710-1790	66-2	11	.065	HCN (101)	3	5	
7/21-2	FUND	1770-1890	.5-2	9	.057	HCN (001)	2	1	0.0021
7/22	FUND	1790-1890	.5-2	9	.057	HCN (101)	3	4	
7/25	FUND	1890-1970	1-64	9	.058	HCN (001)	2	1	0.0026
7/26	FUND	1890-1970	1-64	9	.058	HCN (101)	3	4	
						HCN (001)	2	4	0.0031
						HCN (101)	3	3	
						HCN (001)	2	3	0.0025
						HCN (101)	3	3	
						HCN (001)	2	3	0.0027
						HCl (2-0)	3	3	
						HCN (101)	3	2	0.0027
						HCl (2-0)	3	3	
						HCl (2-0)	3	3	0.0026
						CO (1-0)	1	80-60	
						HCl (2-0)	3	4	0.0018
						CO (1-0)	1	80-60	

All of the above spectra were recorded with the following conditions: Pathlength, 945 cm; grating, 300 lines/mm; detector, Kodak PbSe E-2; grating rotations, 0.02 and 0.05 degs./min.

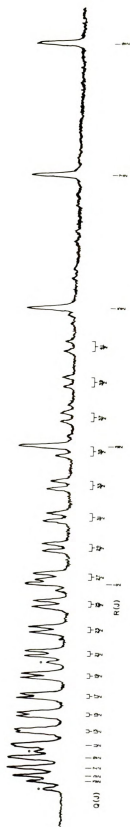
$^{15}\text{N}^{16}\text{O}$ HES

Fig. 5.1. High resolution spectra of the Q-branch region of the 1-0 HES band of $^{15}\text{N}^{16}\text{O}$. Pressure, 75 torr; pathlength, 945 cm; slit-function FWHM, 0.06 cm^{-1} . Lines with circles above them are $^{14}\text{N}^{16}\text{O}$ transitions.

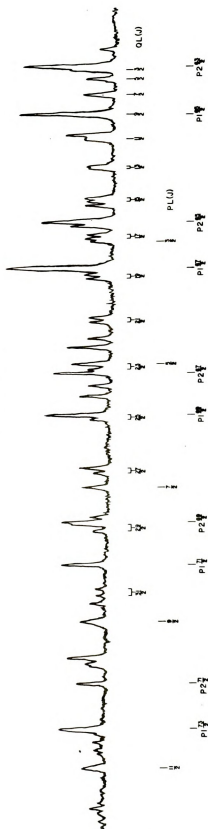
$^{15}\text{N}^{16}\text{O}$ LES

Fig. 5.2. High resolution spectra of the Q-branch region of the 1-0 LES band of $^{15}\text{N}^{16}\text{O}$. Pressure, 70 torr; pathlength, 945 cm; slit-function FWHM, 0.06 cm^{-1} .

is described in Appendix VII-A. Identification of the transitions presented no difficulty.

The "effective" rotational, vibrational and spin-orbit constants may be obtained from the method of combination differences (55) and/or from frequencies. Both of these approaches were used. In each case the appropriate formula was fit to the observed data by the method of least squares using the M. S. U. CDC 3600 computer. Data from all bands for a given isotopic species were fit simultaneously. The least squares subroutine used in all fitting programs gives estimators for the constants and their standard errors. From this the simultaneous confidence intervals (SCI) (56) can be calculated for each constant. On all fits a level of significance of 0.05 was chosen (i.e., a 95% SCI was used).

Combination differences were calculated from the observed frequencies using program DIFF. This program, given in Appendix VII-B, calculates all possible $\Delta_1 F$ and $\Delta_2 F$'s and forms a weighted average of the appropriate components to determine the final values for both the ground and upper state. Because of the statistical nature of the problem, one may use both $\Delta_1 F$ and $\Delta_2 F$'s in determining the constants. Frequencies used in forming the combination differences are the average of the Λ -doublet frequencies.



Effective Energy Expressions

For the $^2\Pi$ state of NO, $L = 1$, $\Lambda = \pm 1$, and $\lambda_v = A_v/B_v \approx 73$. The radical in Eq. (1.17) may therefore be expanded in powers of $(J+\frac{1}{2})^2$. Keeping terms through $(J+\frac{1}{2})^6$ yields:

$$\begin{aligned} T_i^\Lambda(J, v) = & T_e + G(v) - D_v + (-1)^i Q_v/2 \\ & + B_{vi} (J+\frac{1}{2})^2 - D_{vi} (J+\frac{1}{2})^4 + H_{vi} (J+\frac{1}{2})^6 \\ & \pm E_i^\Lambda(J, v) \quad , \end{aligned} \quad (5.1a)$$

where

$$Q_v = A_v - 2B_v - 2B_v^2/A_v + \dots \quad , \quad (5.1b)$$

$$B_{vi} = B_v + D_v + (-1)^i B_v [\lambda_v + 2\lambda_v^2 + \dots] \quad , \quad (5.1c)$$

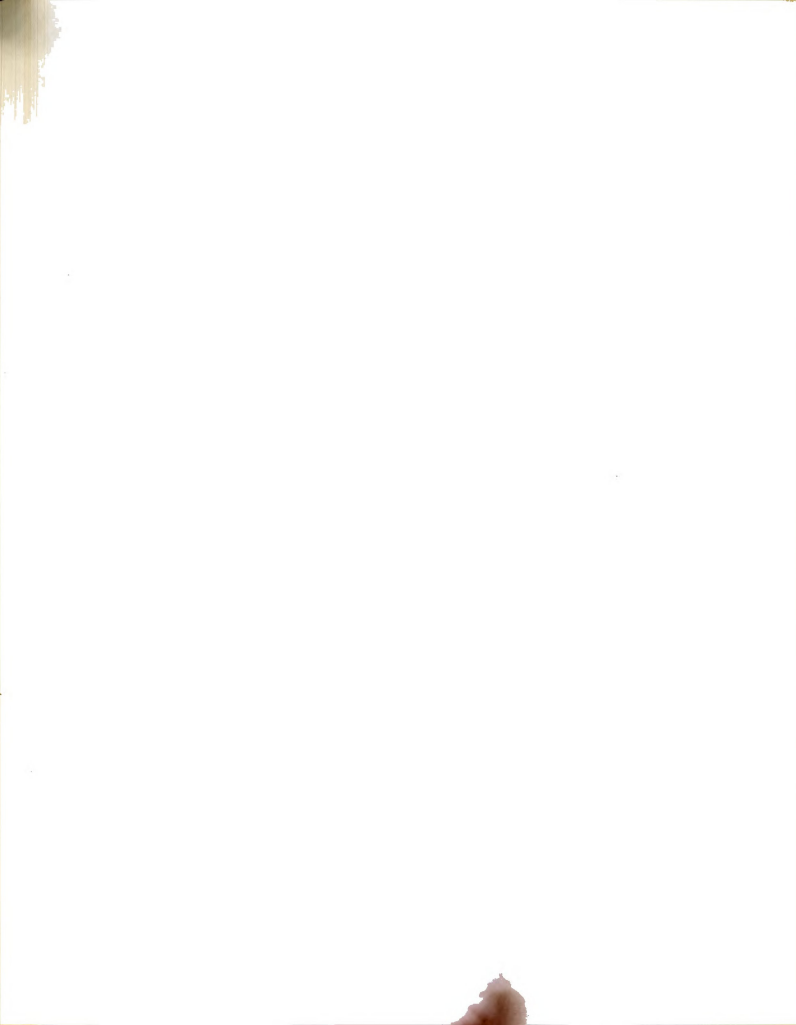
$$D_{vi} = D_v + (-1)^i B_v [\lambda_v^3 + 6\lambda_v^4 + \dots] \quad , \quad (5.1d)$$

$$H_{vi} = (-1)^i B_v [2\lambda_v^5 + 20\lambda_v^6 + \dots] \quad . \quad (5.1e)$$

B_{vi} , D_{vi} and H_{vi} are "effective" rotational constants. The energies in Eq. (5.1a) are essentially those of two simple diatomic molecules with an electronic energy separation of Q_v .

From Eqs. (5.1c), (5.1d) and (5.1e) the "true" rotational constants are:

$$B_v = \frac{B_{v1} + B_{v2}}{2} - D_v \quad (5.2a)$$



$$D_v = \frac{D_{v1} + D_{v2}}{2} \quad (5.2b)$$

$$H_v = \frac{H_{v1} + H_{v2}}{2} \equiv 0 \quad (5.2c)$$

The "effective" rotational and spin-orbit constants were assumed to be linear functions of v , viz.

$$B_{vi} = B_{0i} - \alpha_i v \quad , \quad (5.3a)$$

$$D_{vi} = D_{0i} + \beta_i v \quad , \quad (5.3b)$$

$$H_{vi} = H_{0i} - \gamma_i v \quad , \quad (5.3c)$$

$$A_v = A_0 - \chi v \quad . \quad (5.3d)$$

The expressions for the combination differences and frequencies, including the above assumptions, which were fit are found in Appendix VI-A and VI-B. They are listed there in a form readily adaptable for computer use.

Two methods were used in obtaining the molecular constants. In the first method the ground state combination difference data were first fit, using program ROTCONS given in Appendix VII-C, to determine the "effective" ground state rotational constants. 80 and 76 non-zero weighted GSCD with J-values up to $7\frac{1}{2}$ for $^{14}\text{N}^{16}\text{O}$ and $^{15}\text{N}^{16}\text{O}$ respectively were fit. These ground state constants were then fixed in the frequency fit (using program ALLFIT given in Appendix VII-D) thereafter determining only the "effective" upper state constants. The fits indicated that the upper state "effective" constants were determined less accurately in a fit of the

upper state combination differences than in the fit of frequencies in which the ground state "effective" constants were fixed. For this reason all upper state constants quoted were determined from a fit of frequencies. From preliminary fits it was found that H_{V1} and H_{V2} were equal and opposite to the accuracy of our measurements; consequently they were replaced by a single constant, $H_V' = H_{V2} = -H_{V1}$. The final least squares output from these two fits, for both molecules, is given in Appendix VIII, which includes the observed, predicted and observed minus predicted values for all data points.

In the second method, a frequency fit was made in which all constants, both upper and ground "effective" rotational, spin-orbit and vibrational, were determined simultaneously. The final least squares output from this fit for both molecules is given in Appendix IX.

Effective Rotational Constants

The values of the "effective" rotational constants with their 95% SCI from these two methods are listed in Table 5.2 under Case I and Case II respectively. While the constants overlap in almost all cases, within their 95% SCI, it is still disconcerting that the overall standard deviations of the frequency fits, also listed there, should differ by such an amount. Attempts were made to remove this discrepancy. One of these was the inclusion of an A_J dependence suggested by James (13). While the A_J term was on the verge of significance, it did not improve this situation.



Table 5.2 Effective Constants for NO (cm^{-1}).

Constant	$^{14}\text{N}^{16}\text{O}$		$^{15}\text{N}^{16}\text{O}$	
	Case I	Case II	Case I	Case II
B ₀₁	1.672171 $\pm$ 0.000074*	1.672045 $\pm$ 0.000088	1.613932 $\pm$ 0.00010	1.613844 $\pm$ 0.000093
B ₁₁	1.655021 $\pm$ 0.000084	1.654952 $\pm$ 0.000093	1.597663 $\pm$ 0.00010	1.597583 $\pm$ 0.000095
B ₀₂	1.720020 $\pm$ 0.000086	1.720168 $\pm$ 0.000089	1.658419 $\pm$ 0.00011	1.658526 $\pm$ 0.000086
B ₁₂	1.702053 $\pm$ 0.000091	1.702113 $\pm$ 0.000093	1.641404 $\pm$ 0.00011	1.641479 $\pm$ 0.000089
D ₀₁	(1.16 $\pm$ 0.11) $\times 10^{-6}$	(0.83 $\pm$ 0.11) $\times 10^{-6}$	(1.33 $\pm$ 0.17) $\times 10^{-6}$	(1.15 $\pm$ 0.14) $\times 10^{-6}$
D ₁₁	(1.27 $\pm$ 0.13) $\times 10^{-6}$	(1.06 $\pm$ 0.12) $\times 10^{-6}$	(1.40 $\pm$ 0.17) $\times 10^{-6}$	(1.23 $\pm$ 0.14) $\times 10^{-6}$
D ₀₂	(9.78 $\pm$ 0.12) $\times 10^{-6}$	(10.11 $\pm$ 0.11) $\times 10^{-6}$	(8.83 $\pm$ 0.16) $\times 10^{-6}$	(9.02 $\pm$ 0.12) $\times 10^{-6}$
D ₁₂	(9.71 $\pm$ 0.13) $\times 10^{-6}$	(9.91 $\pm$ 0.12) $\times 10^{-6}$	(8.80 $\pm$ 0.16) $\times 10^{-6}$	(8.96 $\pm$ 0.12) $\times 10^{-6}$
H ₀ [†]	(7.26 $\pm$ 0.51) $\times 10^{-10}$	(8.80 $\pm$ 0.53) $\times 10^{-10}$	(6.09 $\pm$ 0.79) $\times 10^{-10}$	(6.93 $\pm$ 0.68) $\times 10^{-10}$
H ₁ [†]	(7.07 $\pm$ 0.58) $\times 10^{-10}$	(8.03 $\pm$ 0.58) $\times 10^{-10}$	(6.09 $\pm$ 0.79) $\times 10^{-10}$	(6.93 $\pm$ 0.68) $\times 10^{-10}$
α_1	0.017151 $\pm$ 0.000040	0.017093 $\pm$ 0.000029	0.016269 $\pm$ 0.000023	0.016261 $\pm$ 0.000018
α_2	0.017968 $\pm$ 0.000031	0.018055 $\pm$ 0.000029	0.017015 $\pm$ 0.000025	0.017048 $\pm$ 0.000021
β_1	(11.3 $\pm$ 6.1) $\times 10^{-8}$	(23.19 $\pm$ 4.8) $\times 10^{-8}$	(7.6 $\pm$ 1.9) $\times 10^{-8}$	(8.2 $\pm$ 1.5) $\times 10^{-8}$
β_2	(-6.5 $\pm$ 5.3) $\times 10^{-8}$	(-20.14 $\pm$ 4.6) $\times 10^{-8}$	(-3.6 $\pm$ 2.3) $\times 10^{-8}$	(-6.4 $\pm$ 1.9) $\times 10^{-8}$
γ [†]	(0.19 $\pm$ 0.28) $\times 10^{-10}$	(0.77 $\pm$ 0.24) $\times 10^{-10}$	-	-
No. pts. fit	208	208	183	183
s.d.(line fit)	0.0065	0.0035	0.0059	0.0035

* 95% Simultaneous Confidence Intervals

Our values of the "effective" rotational constants from Case I are listed in Table 5.3 along with those of other researchers. Small differences between our constants and others could arise from the fact that an H_V dependence has been included. In fitting the data this will of necessity affect the values of the other constants.

Rotational Constants

The rotational constants for both molecules were calculated from Eqs. (5.2a) and (5.2b) and are given in Table 5.4. In this Eqs. (1.11) and (1.12) have been used. These rotational constants, determined from Case I and Case II "effective" constants, agree to well within their 95% SCI.

Spin-Orbit Constants

The constants Q_0 and χ were determined directly from the frequency fit since satellite data is included. From the values of Q_0 and B_0 , A_0 can be obtained by solution of the simple quadratic (obtained by neglecting terms of order $2B_V^3/A_V^2 \approx 0.0006 \text{ cm}^{-1}$ and higher) of Eq. (5.1b). Table 5.5 lists the values of A_0 , A_1 , A_e and χ_e obtained. It is seen from this that the spin-orbit constants from Case I are the same, within their 95% SCI, for both isotopes, as are those from Case II. Our values for A_0 and A_1 should be compared with those of James (13) for $^{14}\text{N}^{16}\text{O}$ ($A_0 = 123.16 \pm 0.02 \text{ cm}^{-1}$ and $A_1 = 122.91 \pm 0.02 \text{ cm}^{-1}$).

Table 5.3 Comparison of Effective Constants for NO (cm^{-1}).

Effective Constants of $^{14}\text{N}^{16}\text{O}$ (cm^{-1}).						
Constant	Shaw (6)	Olman, et.al. (11)	James, Thibault (13)	Meyer, et.al. (14)	Microwave (5,9)	This Work
B ₀₁	1.6733	1.67233	1.67229	1.67223	1.67186	1.67217
B ₀₂	1.7200	1.72012	1.72014	1.72002	1.72024	1.72002
B ₁₁	1.6561		1.65509			1.65502
B ₁₂	1.7023		1.70225			1.70205
D ₀₁ ×10 ⁶	2.8	1.6	0.77	1.5	1.13	1.2
D ₀₂ ×10 ⁶	9.1	9.5	10.7	9.3	10.6 (c)	9.8
D ₁₁ ×10 ⁶	2.8		0.75			1.3
D ₁₂ ×10 ⁶	9.1		10.7			9.7
H ₀₁ ×10 ¹⁰			-21. (c)			-7.3
H ₀₂ ×10 ¹⁰			21. (c)			7.3

Effective Constants of $^{15}\text{N}^{16}\text{O}$ (cm^{-1}).				
Constant	Microwave (5)	Olman, et al. (11)	Griggs, et.al. (16)	This Work
B ₀₁	1.61362	1.61419	1.61423	1.61393
B ₀₂	1.65745	1.65846	1.65779	1.65842
B ₁₁			1.59793	1.59766
B ₁₂			1.64079	1.64140
D ₀₁ ×10 ⁶	0.57	1.9	2.5	1.3
D ₀₂ ×10 ⁶	8.7 (c)	8.4	7.5	8.8
D ₁₁ ×10 ⁶			2.5	1.4
D ₁₂ ×10 ⁶			7.5	8.8
H ₀₁ ×10 ¹⁰				-6.1
H ₀₂ ×10 ¹⁰				6.1

(c) Indicates a calculated value.

Table 5.4 Rotational Constants for NO (cm^{-1}).

Constant	$^{14}\text{N}^{16}\text{O}$		$^{15}\text{N}^{16}\text{O}$	
	Case I	Case II	Case I	Case II
B_0	$1.696090 \pm 0.000056^*$	1.696101 ± 0.000063	1.636170 ± 0.000075	1.636175 ± 0.000061
B_1	1.678537 ± 0.000063	1.678527 ± 0.000066	1.619528 ± 0.000075	1.619526 ± 0.000065
D_0	$(5.47 \pm 0.08) \times 10^{-6}$	$(5.47 \pm 0.08) \times 10^{-6}$	$(5.08 \pm 0.12) \times 10^{-6}$	$(5.09 \pm 0.10) \times 10^{-6}$
D_1	$(5.49 \pm 0.09) \times 10^{-6}$	$(5.48 \pm 0.08) \times 10^{-6}$	$(5.10 \pm 0.12) \times 10^{-6}$	$(5.09 \pm 0.10) \times 10^{-6}$
B_e	1.704867 ± 0.000057	1.704888 ± 0.000064	1.644491 ± 0.000077	1.644499 ± 0.000063
α_e	0.017554 ± 0.000025	0.017574 ± 0.000020	0.016642 ± 0.000017	0.016649 ± 0.000014
D_e	$(5.46 \pm 0.09) \times 10^{-6}$	$(5.46 \pm 0.08) \times 10^{-6}$	$(5.07 \pm 0.12) \times 10^{-6}$	$(5.08 \pm 0.10) \times 10^{-6}$
β_e	$(2.4 \pm 3.9) \times 10^{-8}$	$(1.5 \pm 3.3) \times 10^{-8}$	$(2.0 \pm 1.5) \times 10^{-8}$	$(0.8 \pm 1.2) \times 10^{-8}$
r_e	1.15063 ± 0.00004	1.15062 ± 0.00004	1.15062 ± 0.00004	1.15061 ± 0.00004

* 95% Simultaneous Confidence Intervals



Table 5.5 Spin-Orbit Constants for NO (cm^{-1}).

Constant	$^{14}\text{N}^{16}\text{O}$		$^{15}\text{N}^{16}\text{O}$	
	Case I	Case II	Case I	Case II
A_0	$123.2089 \pm 0.0049^*$	123.1881 ± 0.0057	123.2030 ± 0.0043	123.1881 ± 0.0052
A_1	122.9521 ± 0.0049	122.9466 ± 0.0057	122.9541 ± 0.0043	122.9459 ± 0.0052
A_e	123.337 ± 0.011	123.3089 ± 0.0090	123.3274 ± 0.0085	123.3092 ± 0.0079
x_e	0.2568 ± 0.0091	0.2415 ± 0.0069	0.2489 ± 0.0073	0.2422 ± 0.0059

* 95% Simultaneous Confidence Intervals

Table 5.6 Isotopic Calculations for $^{15}\text{N}^{16}\text{O}$ (cm^{-1}).

Constant	$^{15}\text{N}^{16}\text{O}$ (obs)		$^{15}\text{N}^{16}\text{O}$ (calc)	
	Case I	Case II	Case I	Case II
B_e	$1.644491 \pm 0.000077^*$	1.644499 ± 0.000063	1.644445 ± 0.000057	1.644465 ± 0.000064
α_e	0.016642 ± 0.000017	0.016649 ± 0.000014	0.016629 ± 0.000025	0.016648 ± 0.000020
D_e	$(5.07 \pm 0.12) \times 10^{-6}$	$(5.08 \pm 0.10) \times 10^{-6}$	$(5.07 \pm 0.09) \times 10^{-6}$	$(5.08 \pm 0.08) \times 10^{-6}$

* 95% Simultaneous Confidence Intervals

Lambda Doubling Constants

A least squares fit to determine the Λ -doubling constants was also performed for each molecule. The expressions which were fit (using program LAMCON given in Appendix VII-E) are given in Appendix VI-C. Doublet separations from both the HES and LES were used. The least squares output for both isotopes is given in Appendix X. Values for these constants (cm^{-1}) are:

	This Work		Microwave (5)	
	$^{15}\text{N}^{16}\text{O}$	$^{14}\text{N}^{16}\text{O}$	$^{15}\text{N}^{16}\text{O}$	$^{14}\text{N}^{16}\text{O}$
$p_{\Lambda} \times 10^3$	$5.672 \pm 0.058^*$	5.828 ± 0.063	5.686	5.876
$q_{\Lambda} \times 10^5$	3.9 ± 1.1	4.6 ± 1.1	2.4	3.84
No. pts. fit	29	41		
Std. dev.	0.0028	0.0043		

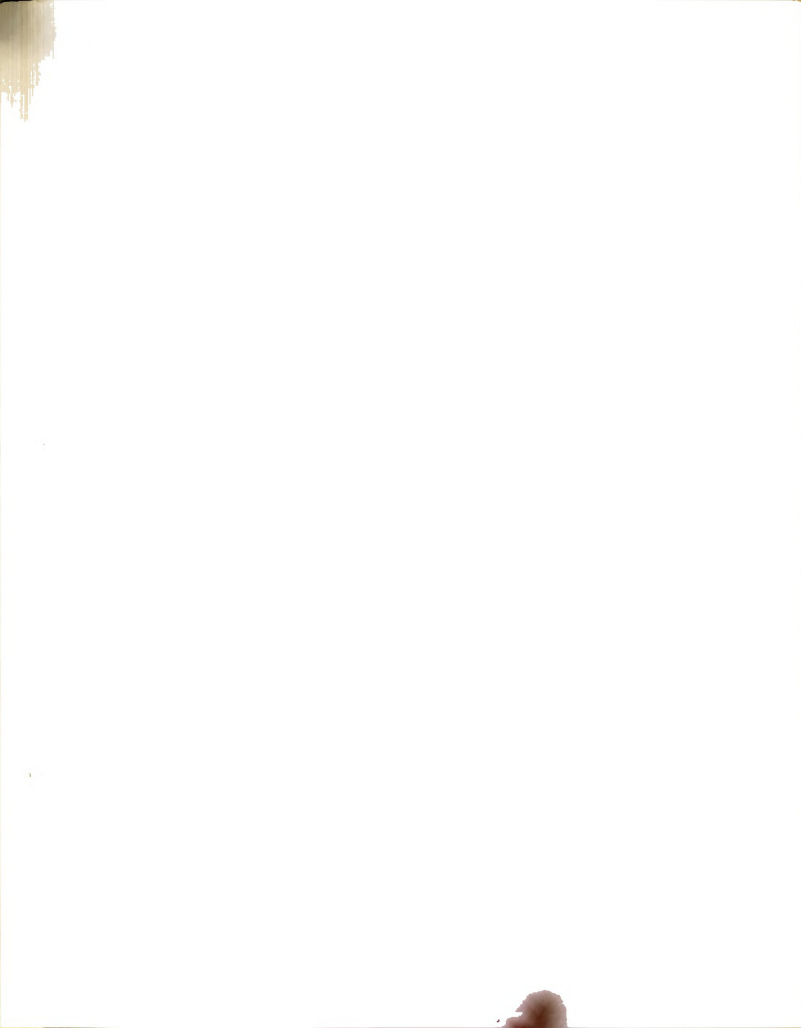
* 95% Simultaneous Confidence Intervals

The values for p_{Λ} agree very well with those obtained from microwave measurements. While the values for q_{Λ} do not overlap theirs, it should be pointed out that much higher J-values are being fit (e.g., up to $J = 47/2$ for $^{14}\text{N}^{16}\text{O}$ and $J = 41/2$ for $^{15}\text{N}^{16}\text{O}$).

Vibrational Constants

Since only one vibrational transition was observed, only one vibrational constant, $\Delta G(1)$, can be determined. The difference in vibrational term values is:

$$\Delta G(v) \equiv G(v) - G(0) = (\omega_e - \omega_e x_e) v - \omega_e x_e v^2 + \dots \quad (5.4)$$



The values for $\Delta G(1)$ from the two cases, given here for completeness, are:

<u>$^{14}\text{N}^{16}\text{O}$</u>		
	Case I	Case II
$\Delta G(1)$	1875.9872 ± 0.0038	1875.9904 ± 0.0026

<u>$^{15}\text{N}^{16}\text{O}$</u>		
	Case I	Case II
$\Delta G(1)$	1842.9366 ± 0.0030	1842.9378 ± 0.0023

The Case I and Case II values do overlap within their 95% SCI.

Isotopic Calculations

The theoretical relations for rotational and vibrational constants between isotopically related molecules in terms of the reduced mass are:

$$B_e^i = \rho^2 B_e, (\alpha_e)^i = \rho^3 \alpha_e, D_e^i = \rho^4 D_e, \omega_e^i = \rho \omega_e, \quad (5.5)$$

where i refers to the substituted species and $\rho^2 = \mu/\mu^i$, μ being the reduced mass of the normal species. Assuming $^{14}\text{N}^{16}\text{O}$ to be the normal species, Table 5.6 lists observed and calculated values for the isotope $^{15}\text{N}^{16}\text{O}$. A value of $\rho = 0.98211970$ was obtained from the AIP Handbook (57). It is seen that these calculated values agree very well with the observed values.



Discussion

The measurement of the line frequencies used in the analysis is believed to be accurate to $0.003\text{--}0.004\text{ cm}^{-1}$.

The "effective" ground state rotational constants determined from the ground state combination difference data are probably the more meaningful of the two sets. It is generally accepted (58) that fitting combination differences leads to a more accurate determination of these constants than a polynomial fit of the frequencies. In addition, the constants determined in this way will not be affected by perturbations of the upper states, and the ground state is less likely to be affected by perturbations.

The difference between the standard deviation of the frequency fit of Case I and Case II could arise due to the fact that in Case I, the fit is being forced to accept values for several of the constants. The curve obtained by varying the remaining constants may not be able to match the experimental curve as well as when all the constants are varied. It is still possible however, that the accuracy of the present data is sufficient for this difference to be pointing to an inadequacy of the present theory. The difficulty does appear to come in large part from trying to fit the satellite and fundamental data simultaneously. James (13) reported difficulty in using constants determined from the fundamental band to accurately predict the observed HES frequencies. The double set of constants is carried throughout to highlight this difficulty.



It is comforting that the "true" rotational constants (Table 5.4) from the two cases are in good agreement. The values for r_e , which are the same, as expected, for both isotopes, are good to the accuracy stated.

It should be stressed that the spin-orbit constants for the two isotopes are in very good agreement for both Case I and Case II. This indicates that both isotopes have identical electronic structure to the accuracy of the data.

The Q-branches of the fundamental subbands overlap considerably, leaving very few unblended lines. This is due in part to the Λ -doubling in the Q_1 lines which is quite large at high J (e.g., $\sim 0.24 \text{ cm}^{-1}$ at $J = 21/2$). For this reason these Q-branches were not included in any of the fits.

It should be emphasized that the data input to all the fits included the lines from both fundamental subbands together with lines from the HES and LES. For reference, the 95% SCI quoted throughout, are ~ 4 times the commonly used standard errors of the coefficients.



CHAPTER 6

ZEEMAN ANALYSIS

In general, Zeeman spectra have not been recorded in the infrared because the resolution was not sufficient to show the individual ΔM transitions. It happens that the splittings for the 2-subband of both $^{14}\text{N}^{16}\text{O}$ and $^{15}\text{N}^{16}\text{O}$ are sufficiently large and the experimental conditions such that for small J-values the extreme components of the transitions could be resolved and their splittings measured. Fig. 7.6 shows Zeeman patterns for the P-branches of the 1- and 2-subbands for low J-values. In Fig. 6.1a the observed Zeeman spectra for the $P_2(5/2)$ line of the (1-0) band of $^{14}\text{N}^{16}\text{O}$ at five different magnetic fields are shown. The patterns for $^{15}\text{N}^{16}\text{O}$ are not significantly different and hence are not reproduced.

The magnetic fields producing these patterns were obtained from an air-core, water cooled solenoid built by the Magnion Corporation. This solenoid is capable of producing fields up to 6800 gauss. It has a central core diameter of seven inches and is forty-eight inches long. Over the region containing the absorption cell, the field is homogeneous to within $\pm 2\%$.



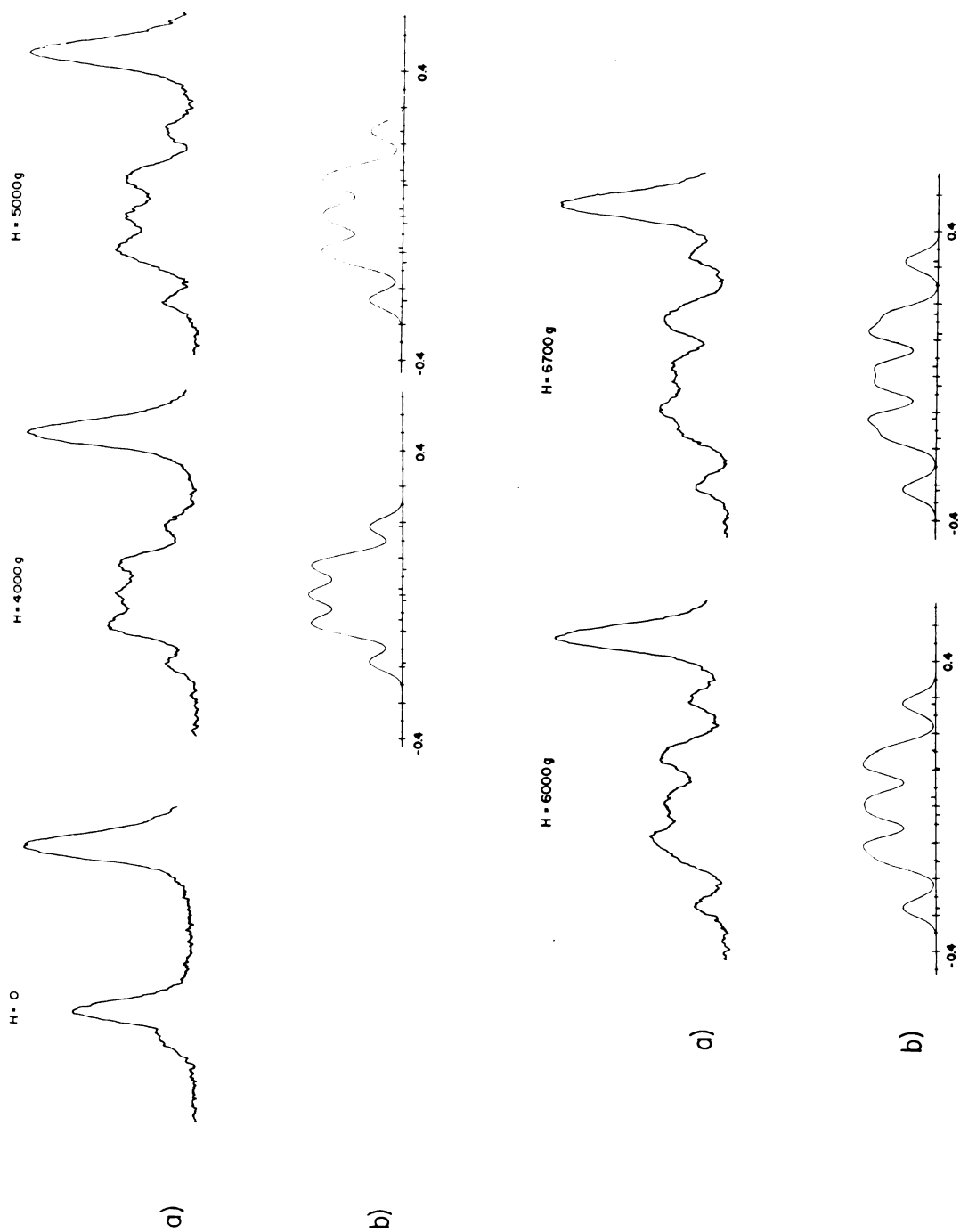


Fig. 6.1. a) Observed Zeeman spectra for the 1-0 band, $P_2(5/2)$ line of $^{14}\text{Ni}^{60}$ as a function of field. Pressure, 4 torr; pathlength, 315 cm; slit-function FWHM, 0.056 cm^{-1} . b) Predicted Zeeman spectra for the same conditions as in a).

From the work of Chapters 2 and 3 the theoretical Zeeman patterns can be predicted. Figure 6.1b shows the predicted Zeeman pattern for the $P_2(5/2)$ transition for the same fields as above. (These were obtained from program PLOTPUN given in Appendix VII-H.) The central components of these transitions overlap considerably; however, the two outermost components appear as single lines.

Measurements of the splittings of the components of the $P_2(5/2)$ and $R_2(3/2)$ lines from the zero field position were made for both $^{14}\text{N}^{16}\text{O}$ and $^{15}\text{N}^{16}\text{O}$. Table 6.1 lists the observed and predicted values (predicted from program ZEEPUN, Appendix VII-G) of these splittings for the various field conditions. The uncertainty in measurement is probably no greater than 0.004 cm^{-1} ; however, the field and therefore the splitting uncertainty ranges between 0.9 and 1.5%. The observed and predicted values agree reasonably well. Microwave measurements of these splittings (58, 59, 60) are more accurate, but the above agreement is good enough so that the interpretation of the observed pattern is certainly correct.

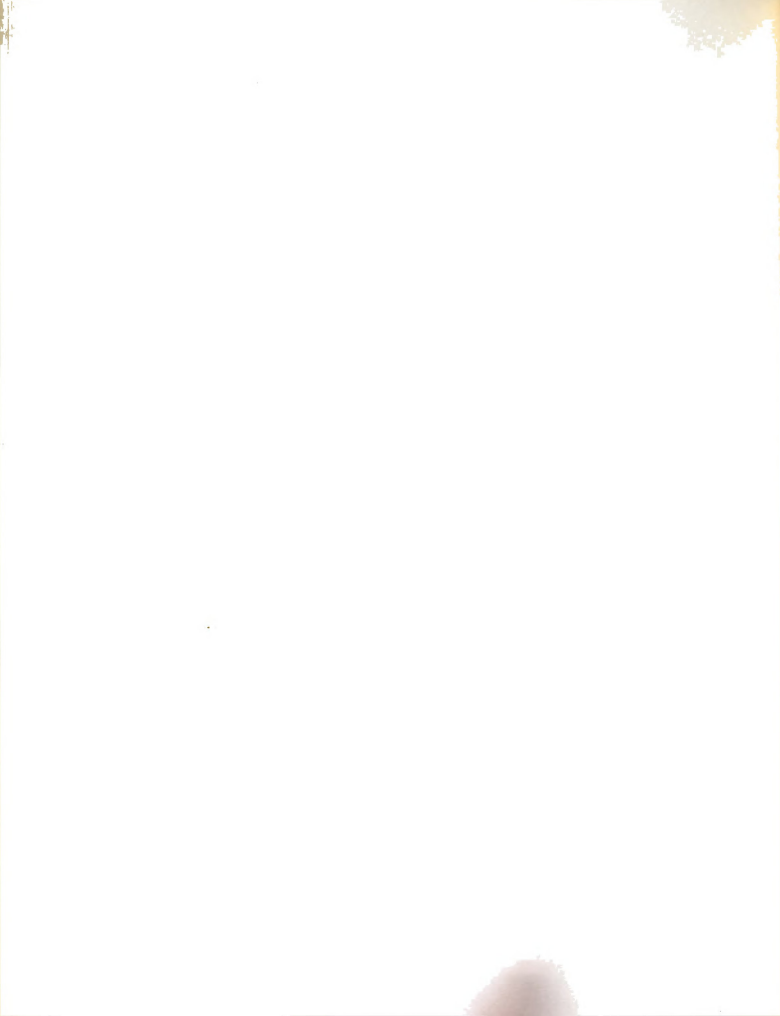


Table 6.1 Zeeman Splittings for the (1-0),
 $P_2(5/2)$ and $R_2(3/2)$ Lines of $^{14}\text{N}^{16}\text{O}$ and $^{15}\text{N}^{16}\text{O}$
as a Function of Field.

		Splittings ^a			
		$P_2(5/2)$		$R_2(3/2)$	
		<u>Obs.</u>	<u>Calc.</u>	<u>Obs.</u>	<u>Calc.</u>
FIELD	(Gauss)				
$^{14}\text{N}^{16}\text{O}$	4000	0.3807	0.3764	--	--
	5000	0.4785	0.4704	0.4784	0.4702
	6000	0.5718	0.5644	0.5648	0.5642
	6700	0.6398	0.6304	0.6328	0.6300
$^{15}\text{N}^{16}\text{O}$	4000	0.3862	0.3760	--	--
	5000	0.4732	0.4702	0.4806	0.4708
	6000	0.5686	0.5642	0.5693	0.5650
	6700	0.6248	0.6300	0.6350	0.6308

a) Separation between the most extreme Zeeman components in cm^{-1} .



CHAPTER 7

MAGNETIC ROTATION ANALYSIS

From October 7-27, 1966, quite an extensive series of magnetic rotation spectra were run on the 1-0 band of both $^{14}\text{N}^{16}\text{O}$ and $^{15}\text{N}^{16}\text{O}$ as a function of pressure, path length, field and polarizer angle. This included a look at the HES of $^{14}\text{N}^{16}\text{O}$. Figures 7.1, 7.2, 7.3, 7.4 and 7.5 summarize the main features of these spectra. The experimental arrangement used in obtaining them is described in Chapter 8.

Most features in Figs. 7.1 - 7.4 have been given a qualitative explanation. The opposite rotations of the 1- and 2-subbands of Fig. 7.4 has been observed and accounted for by Mann and Hause (62) and by Aubel and Hause (63). A general explanation for the intensity minimum of the P_2 and R_2 lines near $J = 9/2$, visible in Figs. 7.1 - 7.4, was also given by the latter. The doublet structure seen in the lines in Figs. 7.1 and 7.2 has also been observed by Robinson (64) who simply attributed the occurrence to absorption from a background of non-uniform intensity.

A semi-quantitative description of the above features has been attempted. Using the M. S. U. CDC 3600 computer the numerical integrations of Eqs. (4.14), (4.16a) and (4.17) were carried out to predict the magnetic rotation signal.



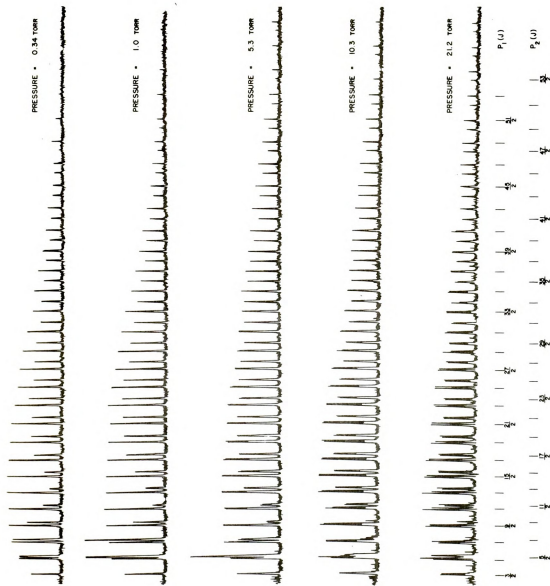


Fig. 7.1. Magnetic rotation spectra of the 1-0 band, p-branch of $1N_2O$ as a function of pressure. These were recorded with a magnetic field strength of 6000 gauss, a pathlength of 315 cm, and a slit-function FWHM of 0.1 cm^{-1} .



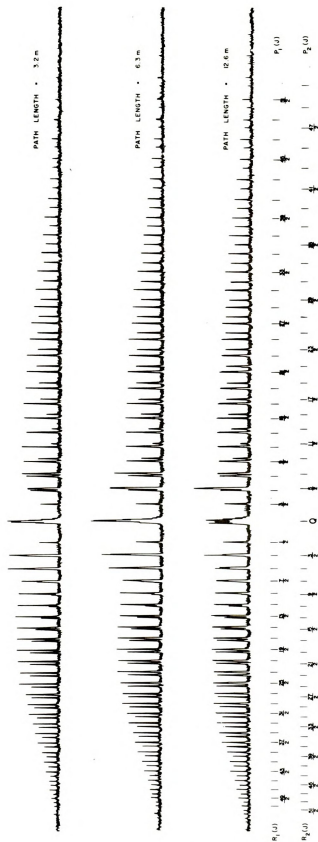


Fig. 7.2. Magnetic rotation spectra of the 1-0 band of $^{14}\text{N}^{16}\text{O}$ as a function of pathlength. These were recorded with a magnetic field strength of 6000 gauss, a pressure of 1 torr, and a slit-function FWHM of 0.1 cm^{-1} .

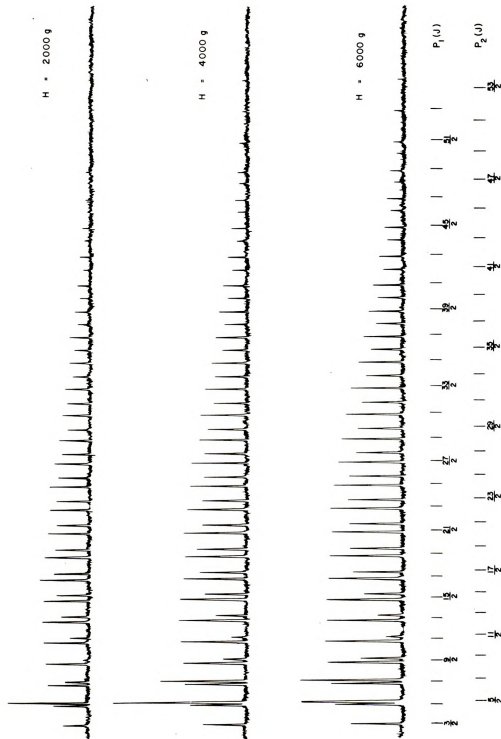


Fig. 7.3. Magnetic rotation spectra of the 1-0 band, P-branch of $^{14}\text{N}^{16}\text{O}$ as a function of magnetic field strength. These were recorded with a pressure of 1 torr, a pathlength of 315 cm and a slit-function FWHM of 0.1 cm^{-1} .

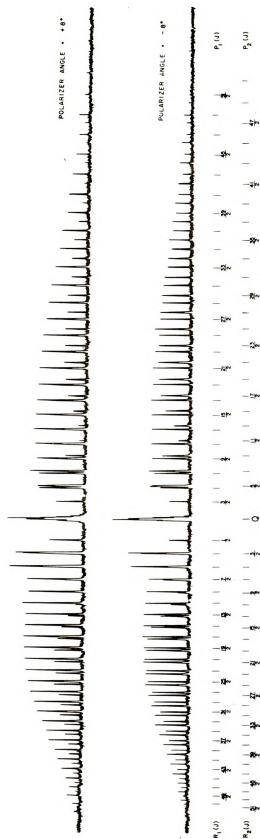


Fig. 7.4. Magnetic rotation spectra of the 1-0 band of $^{14}\text{N}^{16}\text{O}$ as a function of polarizer angle. These were recorded with a field strength of 6000 gauss, a pressure of 1 torr, a path-length of 315 cm and a slit-function FWHM of 0.1 cm^{-1} . The 1- and 2-subband lines exhibit positive and negative rotation respectively.

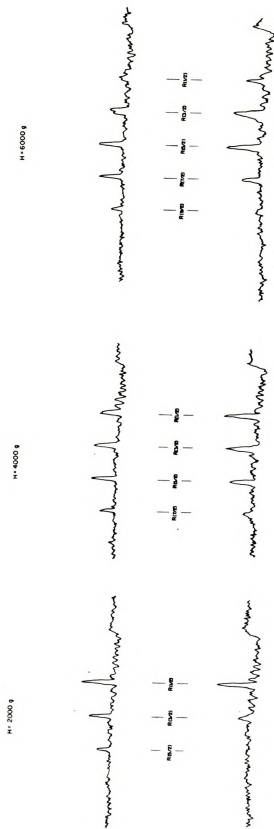


Fig. 7.5. Magnetic rotation spectra of the R-branch region of the 1-0 HES band of $^{14}\text{Ni}^{16}\text{O}$ as a function of field and pressure. The pressures for the upper and lower spectra are 200 and 400 torr respectively. Pathlength, 315 cm; slit-function FWHM, 0.17 cm^{-1} .

at
r
B
tl
of
to
su
sha
the
and
sed
that

These predictions also give a clearer picture of the whole magnetic rotation effect. In all calculations it is assumed that the adjacent lines do not add appreciably to the circular birefringence or dichroism. The effect of overlap is considered later. Program PLOTPUN, listed in Appendix VII-H, carried out the necessary computations and plotted the output. Pertinent magnetic rotation parameters which are input are the Doppler HWHM, Lorentz HWHM, spectrometer HWHM, pressure, pathlength, integrated absorption coefficient, polarizer angle, the Zeeman splittings including the Λ -doubling and the relative intensities. The Doppler HWHM for NO at room temperature, calculated from Eq. (4.11) is $\sim 0.002 \text{ cm}^{-1}$. The Lorentz HWHM must be found experimentally. Shaw and Abels (38) have done so for NO and found $\gamma_L \approx 8 \times 10^{-5} \text{ cm}^{-1}/\text{torr}$. It is slightly dependent on the transition. This value has been found to be too low, by at least a factor of 2, to give reasonable matches to the observed magnetic rotation signal. Buckingham and Segal (65) found that a value 4 times larger than this was needed in their predictions for the 3-0 band of NO. The difficulty must be studied in more detail; however, for the time a value increased by 2X will be used. For pressures $\approx 1 \text{ torr}$, $\gamma_D \approx 10\gamma_L$ and one would expect a Doppler lineshape; however, for pressures of $\sim 20 \text{ torr}$, $\gamma_D \approx \gamma_L$. Therefore the intermediate lineshape of Eq. (4.14) was used, which should handle both conditions. A spectrometer HWHM of 0.05 cm^{-1} was used. For general reference this is ~ 3 times smaller than that used by Aubel and Hause (63) for the 2-0 band. This was

possible due to greater dispersion in the region of the 1-0 band coupled with a larger percent magnetic rotation. In the calculations so far, a Gaussian form has been assumed for the spectrometer slit-function. In actual fact, for the mechanical slit-widths used, the slit-function should be more nearly trapezoidal. Eventually careful plots of a narrow emission line should be run for the region of interest and the exact slit-function input to the program. The integrated absorption coefficient was input as calculated from Eq. (2.23). Zeeman splittings were calculated from Eq. (3.7) using program ZEEPUN, and input.

The Zeeman splitting is symmetric to the order of approximation considered here. Fig. 7.6 shows some of the patterns and relative intensities, including the Λ -doubling, for both the 1- and 2-subbands. Each transition is a collection of $(2J+1)$ symmetric doublets, the components of which are characterized by $\Delta M = +1$ and -1 , and which absorb, in equal amounts, right and left circularly polarized light respectively.

The magnetic rotation signal, as will be seen later, is predominantly due to circular birefringence. Typical anomalous dispersion curves for a simple doublet along with the rotation angle θ , are shown in Fig. 7.7. θ is directly proportional to the integrated absorption coefficient, and the calculations show it can attain magnitudes of ~ 70 radians for the 1-0 band. In the central region of the doublet, θ is changing rapidly. One therefore expects $\sin^2 \theta$ to oscillate rapidly between 0 and 1. The frequency of this oscillation

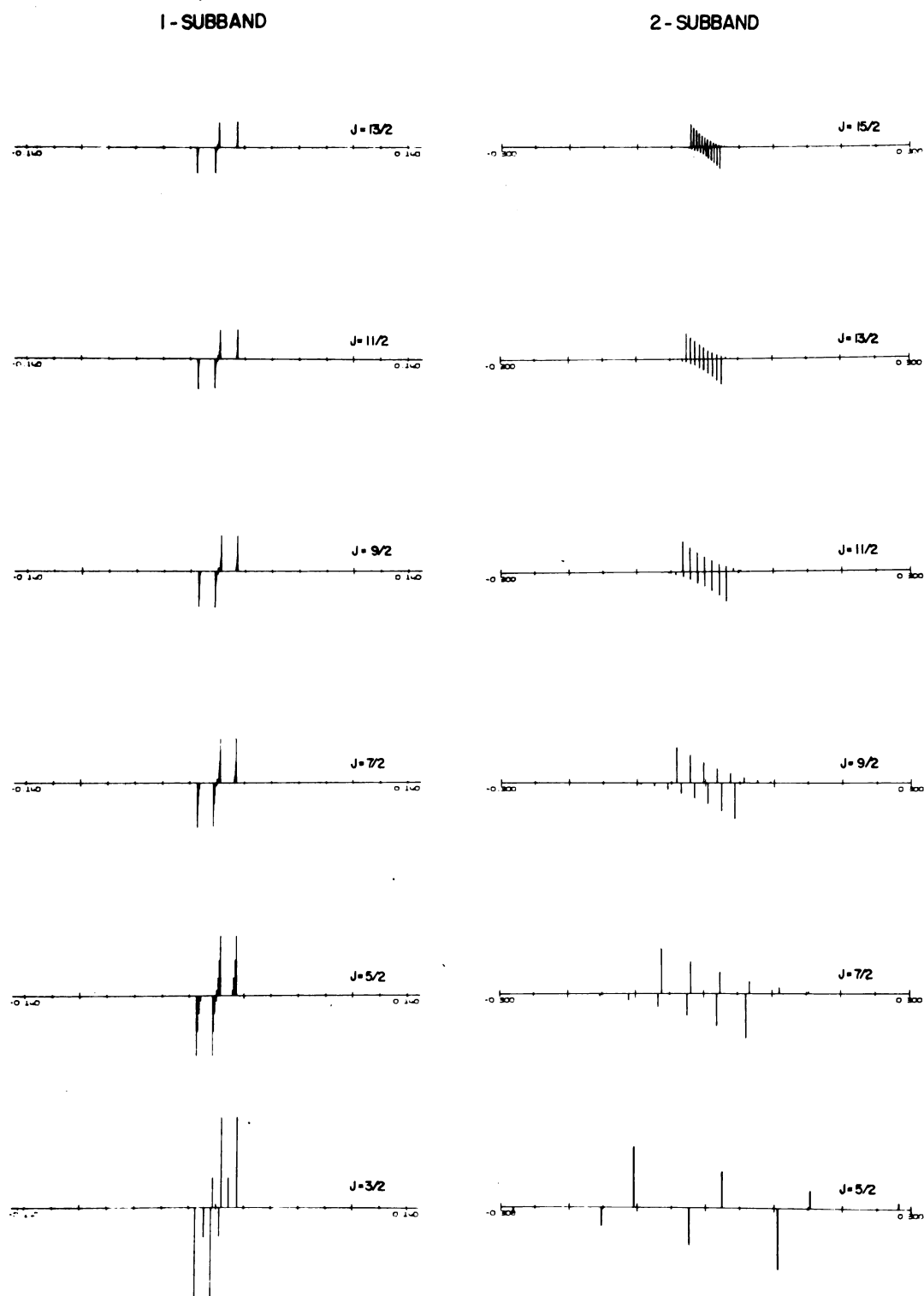


Fig. 7.6. Predicted Zeeman patterns and relative intensities for the 1-0 band, P-branch of $^{14}\text{N}^{16}\text{O}$ for a magnetic field strength of 6000 gauss. Lines drawn upward (downward) correspond to $\Delta M = +1$ (-1) transitions.

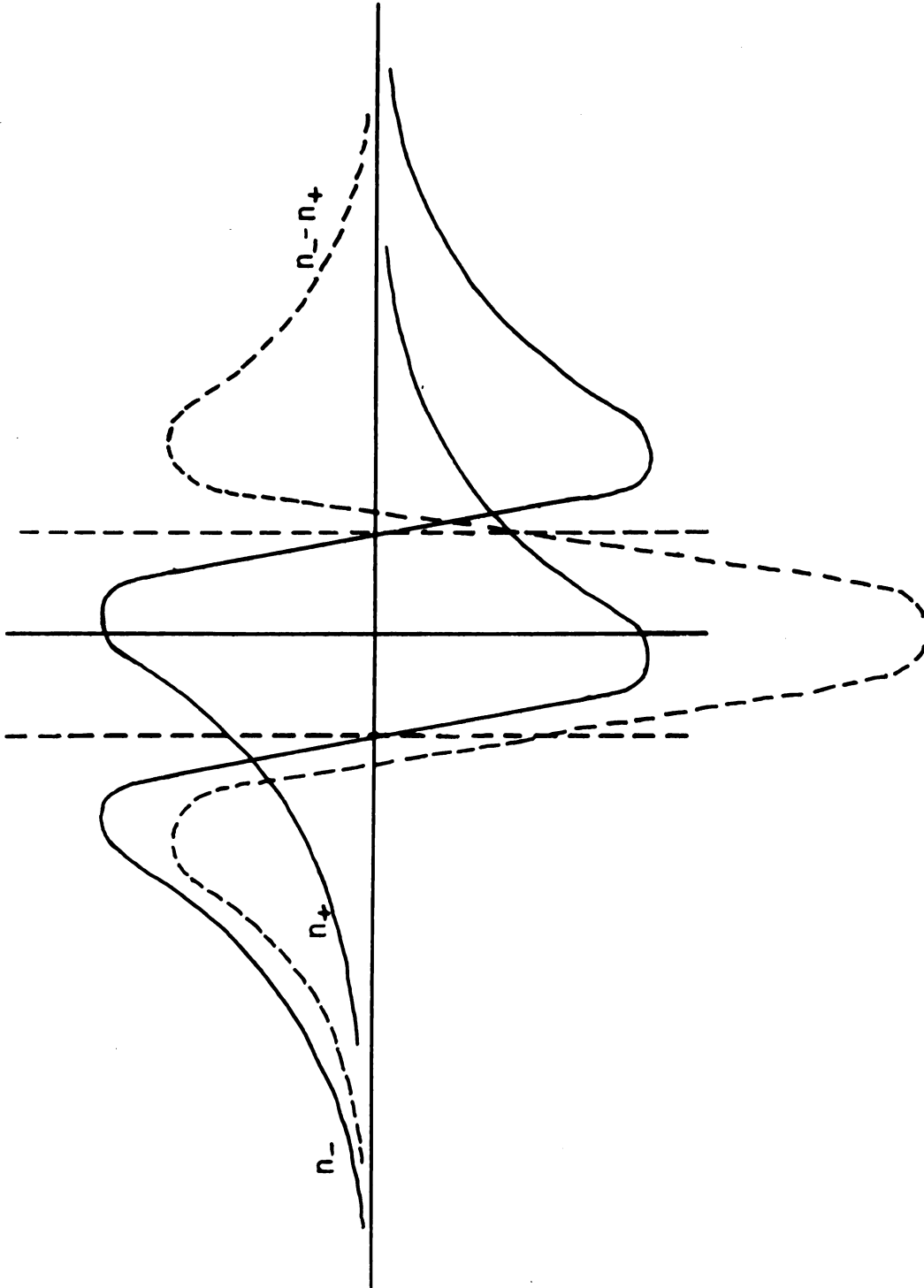


Fig. 7.7. Typical anomalous dispersion curves for a simple Zeeman doublet. n^+ and n^- are the indices of refraction for right and left circularly polarized radiation respectively. The dotted curve is $(n^- - n^+)$ and therefore proportional to θ .



will decrease as one proceeds toward the wing of the transition since there θ changes less rapidly. Finally, as θ becomes less than $\pi/2$, the circular birefringence will decrease to zero. In the extreme wings of the line, the Kramers-Kronig relations (i.e. Eq. (4.16a)) predict $\theta \propto 1/\nu$. The frequency range for $\pi > \theta > 0$ is consequently larger and this last oscillation in the $\sin^2\theta$ term is broad compared to those closer to the line center. Absorption is also taking place throughout this region. The absorption coefficients, for right and left circular polarizations, calculated from Eq. (4.14) and the path lengths used are such that the transmission fractions for even the weakest Zeeman components are zero near the center of the line. However, the absorption coefficient decreases to zero, and the transmission fraction therefore goes to unity, more rapidly than does θ as can be seen from Eq. (4.14). Fig. 7.8 shows the contributions of these various terms for the $P_1(15/2)$ line for one set of conditions. This line, like other l-subband lines, displays nearly a simple doublet Zeeman pattern. The transmission fractions for right and left circular polarizations are shown in Fig. 7.8a. The circular birefringence term (Eq. (4.9b)) will appear, as in Fig 7.8b with nearly zero intensity near the zero field position due to the $\sqrt{T^+T^-}$ coefficient, oscillate to a peak in the wings due to the $\sin^2\theta$ term and finally decrease to zero as $\theta \rightarrow 0$. One notes that there can be no circular birefringence contribution to the magnetic rotation intensity in the absence

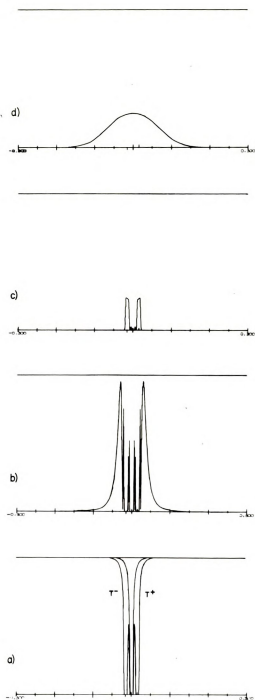


Fig. 7.8. Predictions of the terms making up the magnetic rotation signal of the 1-0 band, $P_1(15/2)$ line of $^{16}\text{N}^{16}\text{O}$. a) Transmission fractions, T^+ and T^- . b) Circular birefringence. c) Circular dichroism. d) Integration of the sum of (b) and (c) over the spectrometer slit-function. Field strength, 6000 gauss; pathlength, 315 cm; pressure, 1 torr; slit-function FWHM, 0.1 cm^{-1} .



of either component of circular polarization.

The circular dichroism pattern, shown in Fig. 7.8c, is obtained directly from Eq. (4.9a). It is seen that this term is non-zero over a comparatively small frequency range and cannot attain a value greater than 0.25. When an integration over the slit-function is performed, it is found that the contribution due to this term is almost negligible.

Finally, Fig. 7.8d shows the MR signal after integration over the spectrometer slit-function. The intensity at line center is ~ 0.25 . Not enough checks of the observed intensity transmitted through parallel polarizer-analyzer were taken. Ultra-violet radiation progressively fogged the first plate of the AgCl polarizer thereby vitiating quantitative intensity measurements; however, earlier measurements indicate that the actual MR signal is ~ 0.30 . The calculated versus observed agreement is reasonable.

As Aubel (63) points out, the magnetic rotation signal for the 1-subband should follow the normal band intensity contour since θ is proportional to the integrated absorption coefficient and all the Zeeman patterns are very nearly the same. Also, as he points out, the angle θ is calculated to be positive in the wings of these lines, thereby giving rise to an enhancement of the magnetic rotation signal for positive polarizer setting.

The 2-subband Zeeman patterns, Fig. 7.6, are quite different from the single doublet character of the 1-subband.



However, after calculating the anomalous dispersion and transmission fraction for each line and performing the appropriate summations, one still ends up with a doublet character as regards right and left circularly polarized light. One expects the 2-subband to have slightly weaker magnetic rotation signals due to both a smaller integrated absorption coefficient and the greater amount of overlap of $\Delta M = +1$ and -1 transitions. A series of plots similar to the ones in Fig. 7.8 have been made for the 2-subband but essentially the same type patterns are obtained. Consequently they have not been included.

Having discussed the makeup of the magnetic rotation signal, let's examine some specific features of Figs. 7.1-7.4.

Doublet Character of MR Lines

As was stated earlier, Robinson (64) qualitatively attributed the effect to simple absorption from a non-uniform background. This is certainly correct; however, going back to Fig 7.8a one can see exactly how it enters. The transmission fraction is zero near the zero field position. If, as was the case in Fig. 7.8, the spectrometer slit-function is much wider than this region of zero transmission, the magnetic rotation signal will appear as a single line. If the absorption coefficient or the pathlength is increased, the region of zero transmission will broaden and may eventually become comparable to the slit-function. At the same



time the angle θ extends its region of non-zero values so that it is always broader than the $\sqrt{T+T}$ term. Upon integration over the slit-function a decrease in magnetic rotation signal will be observed. Figs. 7.9a and 7.9b show predictions for the P_1 and P_2 (15/2) lines at two different pressures which demonstrate this effect. Both the integrated and unintegrated patterns are shown. It should be remarked that the absorption coefficient is increased by an increase in pressure (see Eq. 2.23 and 4.12). This will have a bigger effect than increasing the pathlength since by changing the pressure the lineshape is also altered. An increase in pressure makes the line more nearly Lorentzian, its tail increasing and thereby adding to the doubling effect.

2-Subband Intensity Contour

It was stated earlier that the 2-subband should be slightly weaker than the 1-subband due to a smaller absorption coefficient and greater overlap of right and left circular polarization regions. It is this latter point which is giving rise to the intensity minimums near $J = 9/2$. Consider the 2-subband patterns in Fig. 7.6. If one calculates the ratio of the intensity of the strongest component and the nearest component of opposite polarization one finds a minimum for $J = 9/2$. That is, one can expect a smaller value in the calculation of ϕ in Eq. (4.7) from these components.

This can be extended over all $(2J+1)$ components to predict a smaller magnetic rotation signal from this trans-

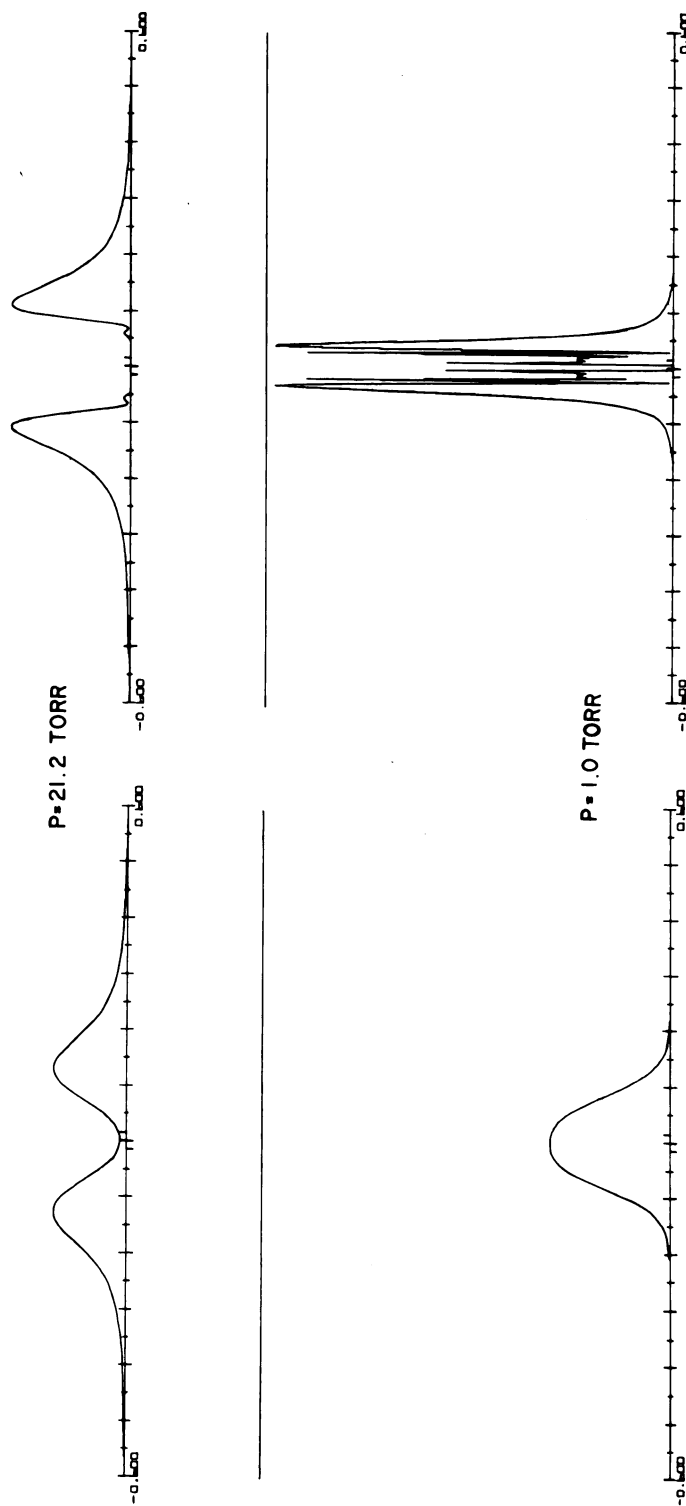


Fig. 7.9a. Predictions of the magnetic rotation signal for the $I-0$ band, $P_1(15/2)$ line at pressures of 1.0 and 10.3 torr. The curves on the left and right are the finite and infinite resolution patterns. Field strength, 6000 gauss; pathlength, 315 cm; slit-function FWHM, 0.1 cm^{-1} .

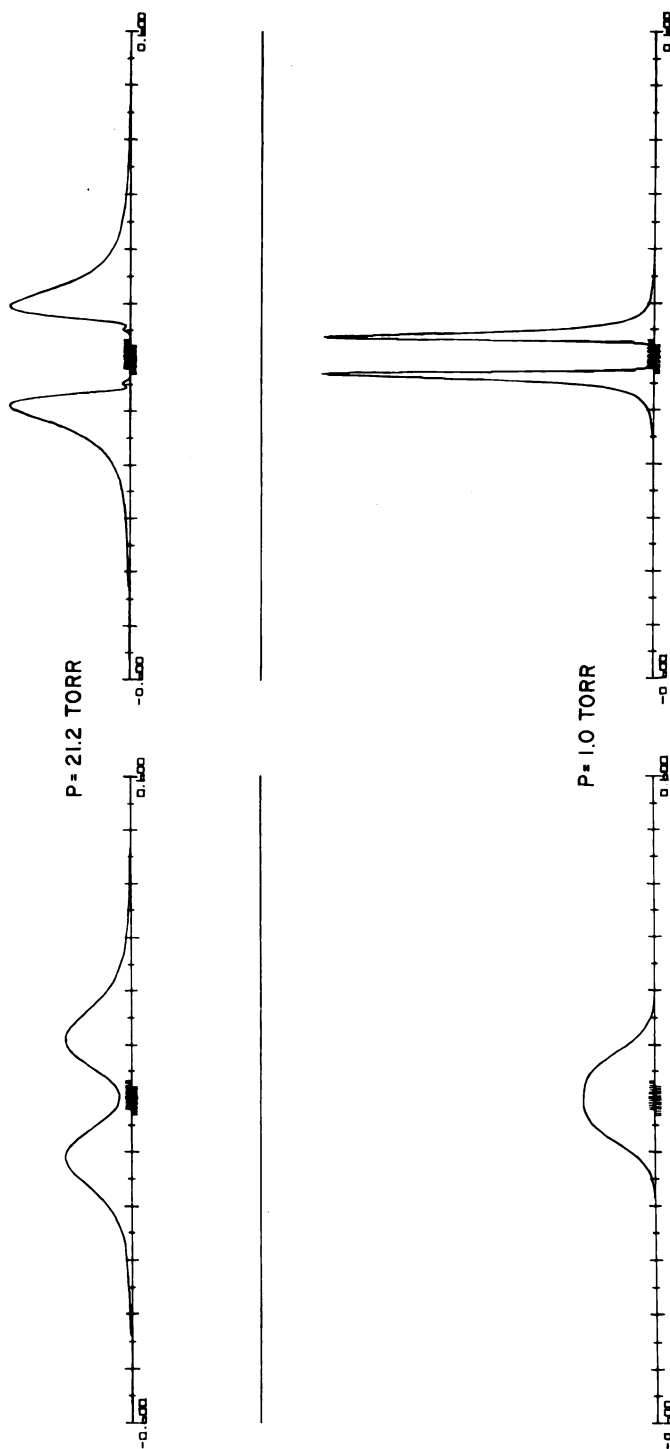


Fig. 7.9b. Predictions of the magnetic rotation signal for the $1-0$ band, $P_2(15/2)$ line at pressures of 1.0 and 10.3 torr. The curves on the left and right are the finite and infinite resolution patterns. Field strength, 6000 gauss; pathlength, 315 cm; slit-function FWHM, 0.1 cm^{-1} .

ition. This is certainly not the entire story however. It is noted that the largest components of the P_2 ($9/2$) line do not lie directly on top of a component of the opposite polarization. In order to get a large cancellation effect these components must overlap within their individual line widths. They are separated by 0.0064 cm^{-1} , thus the absorption coefficient must have a HWHM approaching this to get the maximum cancellation. On the other hand, the $J = 11/2$ components are separated by only 0.0003 cm^{-1} . One might therefore expect the minimum in the magnetic rotation signal to move toward higher J -values for lower pressures, and therefore smaller absorption coefficients. This is borne out by experiment (see Fig. 7.1). By the same line of reasoning, at lower field strengths, where the Zeeman components are closer together, the minimum should move toward lower J -value (see Fig. 7.3). Predictions of the magnetic rotation signal agree very well with experiment as regards this minimum. Fig. 7.10 shows predictions for the P_2 subband for $J = 5/2$ to $15/2$ for two different pressures. It is seen that at the higher pressure the minimum is shifted by one to $J = 9/2$ in agreement with Fig. 7.1.

Directions of Rotation

The subject of the opposing rotations of the 1- relative to the 2-subband has been well explained (63). Let it suffice to say that the predictions made from the theory of Chapter 4 are in complete agreement with the

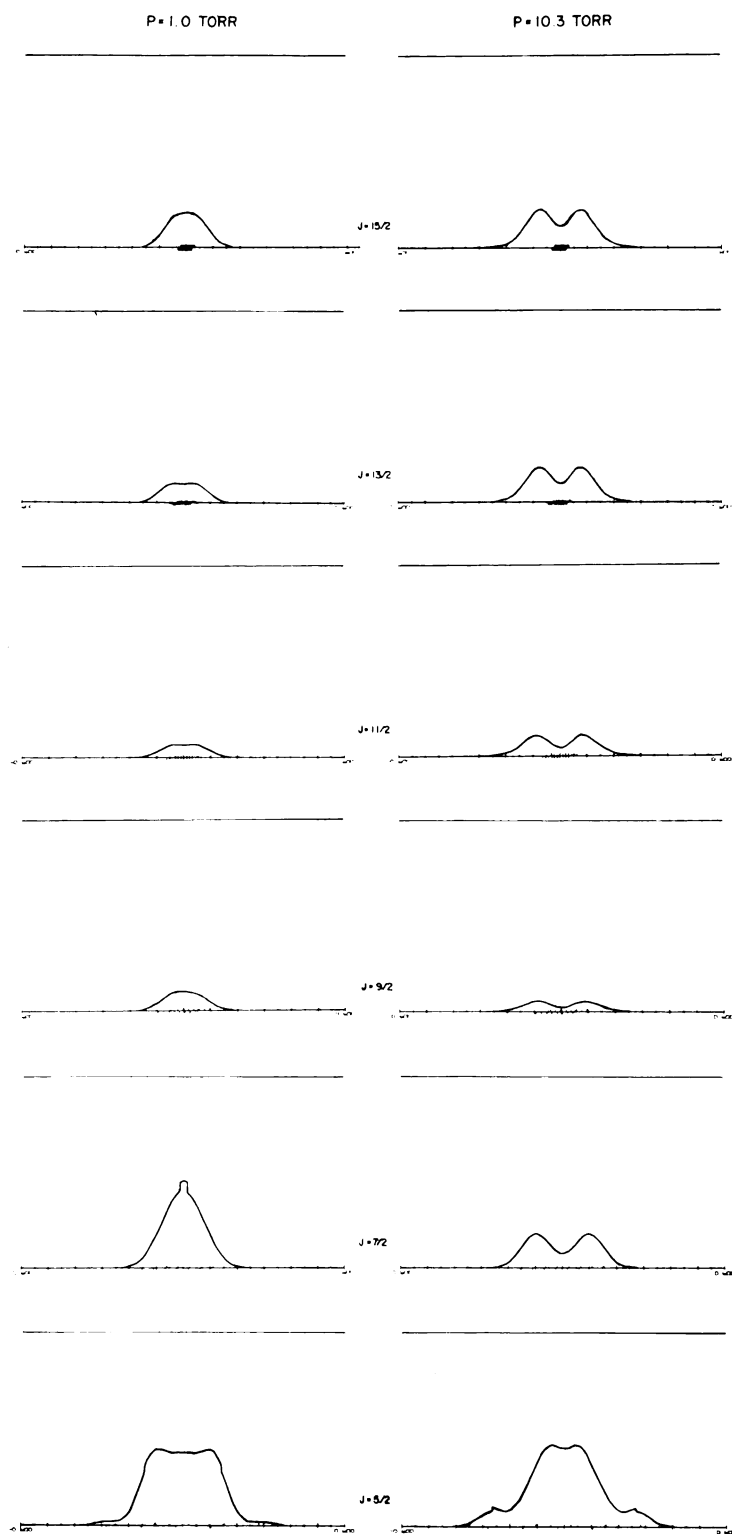


Fig. 7.10. Predictions of the magnetic rotation signal for the 1-0 band, P_2 subband of $^{14}\text{N}^{16}\text{O}$ at pressures of 1.0 and 10.3 torr. Field strength, 6000 gauss; pathlength, 315 cm; slit-function FWHM, 0.1 cm^{-1} .

observation that the rotation is positive (negative) for the 1- (2-)subband. While there are no complete cancellations in the 1-0 band similar to those observed (63) in the 2-0 band, there are nevertheless partial cancellations which become obvious as the absorption is increased. In Fig 7.1 in the region from $J = 7/2$ to $19/2$ for a pressure of 21.2 torr, it is noted that the inner components of the doublets are weaker than the outer. While some of this can be attributed to instrumental factors it is too regular to be explained solely on this basis. It is reasonable to assume that the Lorentz tail on the absorption coefficients for the 1- and 2-subband lines is producing enough overlap to result in partial cancellation of rotations.

Magnetic Rotation Spectra of the HES

Fig 7.5 shows the meager traces of magnetic rotation spectra which were obtained from the $^{14}\text{N}^{16}\text{O}$ HES. A wide range of conditions of pressure, field and pathlength were tried with no better success than this. The transmission for these lines is between 10-15%. There appears to be no one condition of field or pressure which will simultaneously maximize all lines.

The weakness of the observed signals can be attributed to instrumental sensitivity. The failure to observe more lines must be attributed to the combination of line-width ($\gamma_L \approx 0.1 \text{ cm}^{-1}$), Λ -doubling, and Zeeman splittings being right to produce cancellation. This could

explain the non-existence of the Q-branch in Fig. 7.5 as there the overlap of components is great. (For the actual positions of the Q-branch lines see Fig. 5.1.) Fig. 7.11 shows predicted Zeeman patterns, including Λ -doublet splittings, for the HES R-branch lines for J up to $11/2$. It is seen that for $J = 11/2$, and therefore for all higher J -values, the most intense Zeeman components for both Λ -doublet components, are well within the Lorentz halfwidth of the lines. This will result in cancellation which will be less severe at higher values of the field. Also as the pressure, and therefore γ_L , is increased there will be more overlap of the $\Delta M = +1$ and -1 components resulting in smaller signals at higher J -values. This is observed in Fig. 7.5.

Discussion

The calculations, incorporating intensities determined quantum mechanically, inserted into an expression derived using classical dispersion theory and including the effects of a finite resolution spectrometer, have successfully predicted the major features of the magnetic rotation spectrum of the fundamental band of $^{14}\text{N}^{16}\text{O}$. The agreement is not perfect. This is perhaps due partly to the rather crude numerical integrating techniques in which basically the areas of rectangles with equal bases were added for all regions. It is quite conceivable that this led to a distortion of the form of the lineshape and of the rotation angle θ . Nevertheless it would appear that the overall approach is correct.

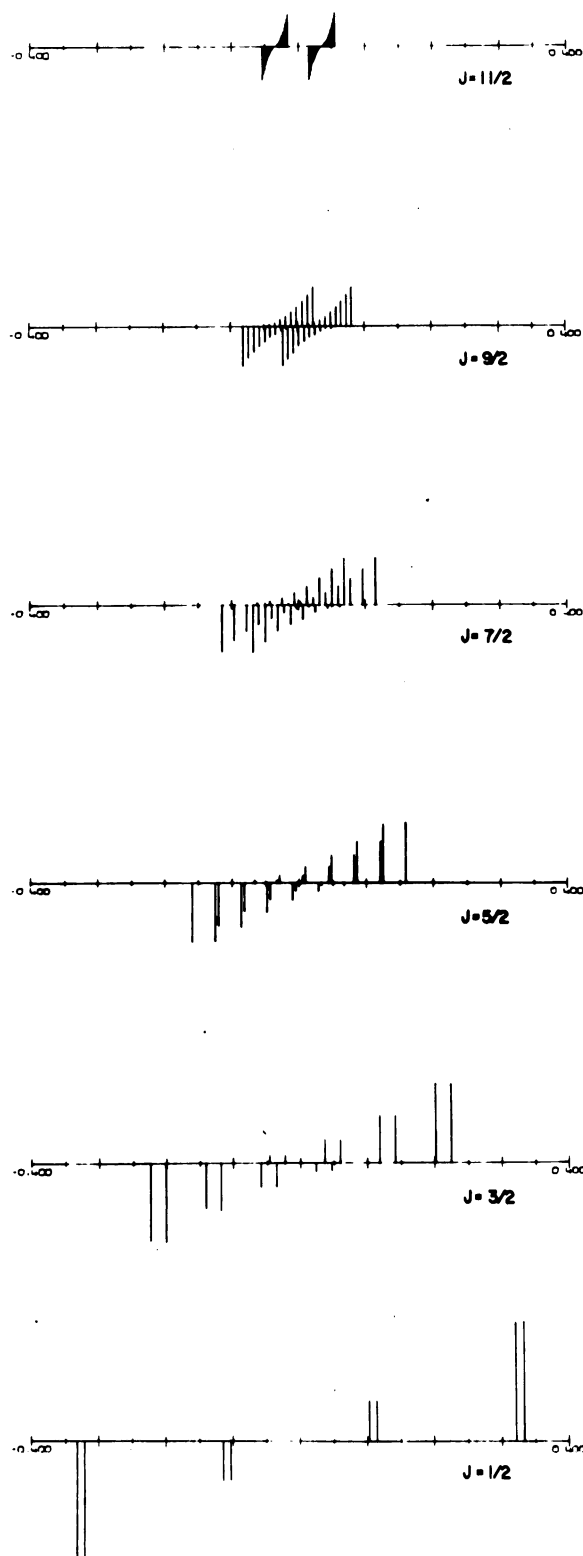
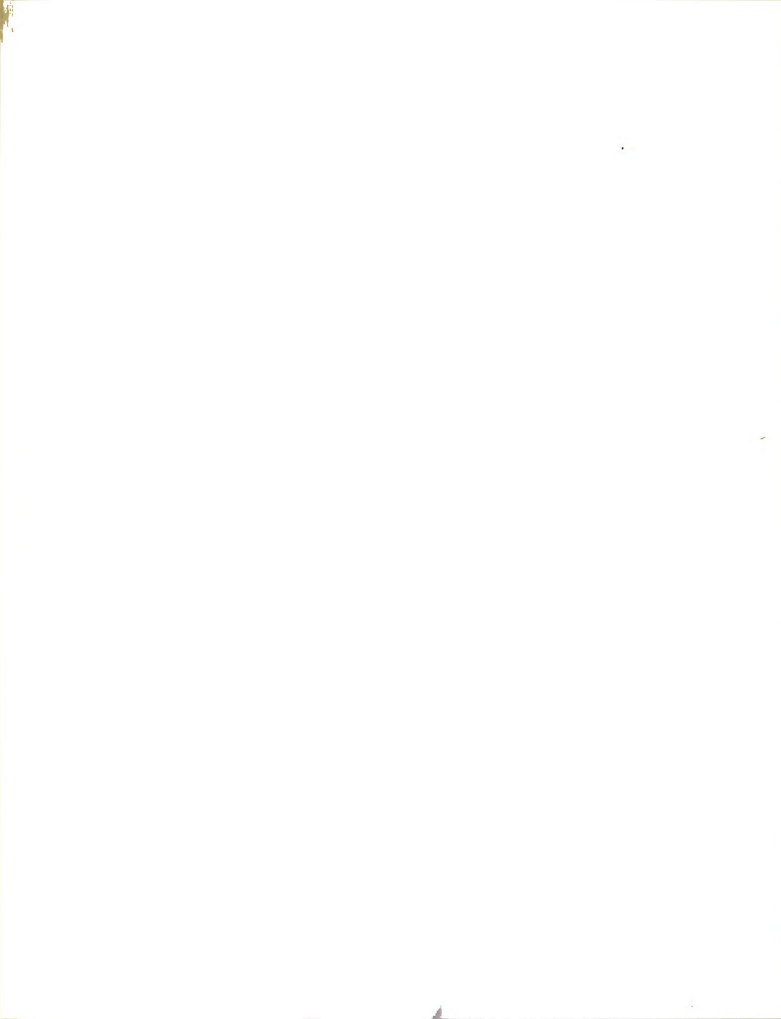


Fig. 7.11. Predicted Zeeman patterns and relative intensities for the 1-0 HES band, R-branch of $^{14}\text{N}^{16}\text{O}$ for a field strength of 6000 gauss. Lines drawn upward (downward) correspond to $\Delta M = +1$ (-1) transitions.



From the plots obtained it appears that the line shape and the exact position of the Zeeman components are the most critical parameters. A change in the integrated absorption coefficient produces a comparatively small change in the magnetic rotation signal.

It would appear that, as regards the determination of any molecular parameters, the magnetic rotation as measured here is of limited usefulness due to the number of superimposed quantities. It has been pointed out (63) however, that the integrated effect as seen here can be used to show the presence of magnetic splittings even when these splittings are more than a factor of 10 below the resolution capabilities of the instrument.

Buckingham and Stephens (21) have mentioned the possibility of reducing the complexity by separating the MCB and MCD terms through application of a "small" alternating magnetic field and using a phase sensitive detector. It is not clear that the magnetic rotation effect would be measurable for "small" fields, however, this possibility should be explored. Eberhardt (66) has also managed to experimentally isolate the quantities θ and ϕ . He accomplished this by chopping the beams with a plane polarizer to isolate the angle of rotation θ , and by chopping with quarter-wave plates to isolate ϕ . These measurements should provide direct determination of molecular transition probabilities. One may have trouble making quarter-wave plates for the near infrared;

however, this approach also has good possibilities. Additional work should be done in obtaining better agreement between theory and experiment for the work presented here. It is still possible that, if the effect can be predicted accurately enough, information on molecular parameters can be extracted.

CHAPTER 8

SPECTROMETER DESCRIPTION

The high resolution infrared instrument used in this work is the result of an evolutionary process beginning with R. H. Noble (67) and including, among others, Brown (68) and Aubel (22). Aubel has given a detailed description of the instrument in its next to present form including alignment procedures.

The modifications which put the instrument in its present form were made during the period from September 1964 to May 1965. An account of these follows. Since the basic alignment procedure has not been altered it has not been included.

Carbon Rod Source

The previously used 300 watt Zr arcs were plagued with a number of difficulties such as; 1) instability in a magnetic field, 2) an envelope which failed to transmit sufficiently well beyond 2.7μ , 3) short and unpredictable outputs and lifetime.

A rod source was developed patterned after the work of Rank (69) and Rao, Spanbauer and Fraley (70) to overcome some of the above difficulties. It is in a water-cooled housing which mounts directly to the tank wall, thereby eliminating

a previous air path. A 2" x 3/16" CaF_2 window presently provides isolation between the rod enclosure and the main vacuum chamber; however, almost any window of similar dimensions could be used. The CaF_2 transmits in excess of 95% out to 7μ . The back end of the enclosure is removable and, as seen in Fig. 8.1, serves as a base for two 1" water-cooled brass posts which deliver current to the rod.

The rod itself is 0.25" x 2" and has an $\sim 13^\circ \text{V}$ 0.125" deep cut longitudinally in it to make it more nearly a black body radiator. National SPK graphite was found to be the most suitable rod material. Electrical contact is made to the rod by means of 2 two-turn coils of #18 copper wire which are pushed over the ends. This is then pushed into two coaxial holes in the 1" posts.

Figure 8.2 is a schematic of the rod power supply. Basically it is a "variac" driven welding transformer operating step-down off the 220 VAC line. Pressure, water and rod breakage cutouts are provided in the system. Typical operating conditions are 410 amps at 7.5 VAC which heats the rod to $\sim 2700^\circ\text{C}$. The supply will furnish 500 amps; however, rod lifetime is cut by about a factor of 3 and output is increased by only $\sim 15\%$. At the normal operating current, the average lifetime is about 20 hrs during which the output is constant. The output is not affected by a magnetic field.

A one atmosphere environment of ultra pure argon is provided during operation which retards evaporation of the rod.

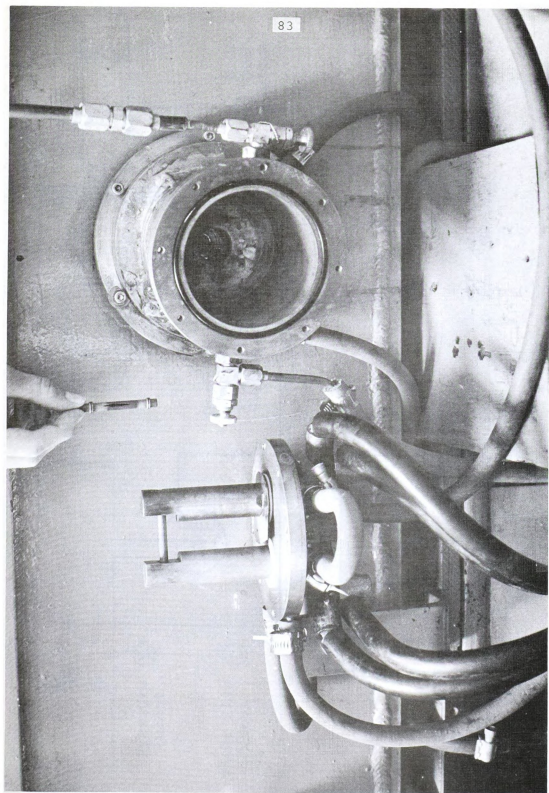


Fig. 8.1. Rod Source.

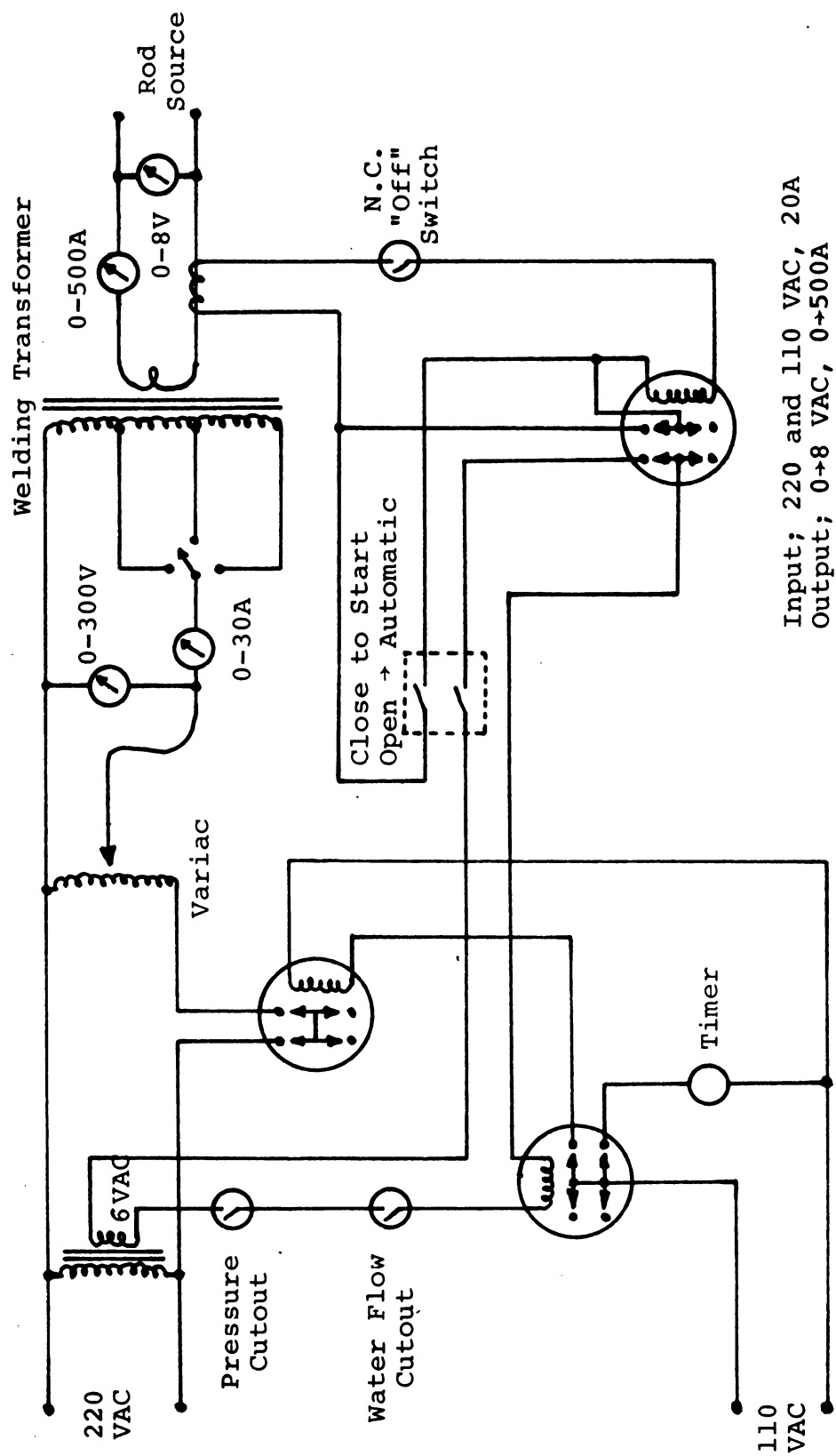


Fig. 8.2. Rod Source Power Supply.

Pressures as high as three atmospheres have been tried with no significant increase in rod life.

It has been found that the rod output at 4400 cm^{-1} is about 30% better than the previously used Zr arcs and very stable throughout its lifetime.

Foreoptics

The basic optical path in the foreoptics has been modified little from the work of Aubel (22), however, a vacuum polarizer assembly has been added to eliminate the last air path in the entire optical train. A false 1" aluminum baseplate has been added, and CaF_2 "windows" are used throughout to allow increased range. The baseplate provides a stable platform for mounting the mirrors and eliminates mirror displacement during tank evacuation. Fig. 8.3 shows the present mirror configuration. Table 8.1 lists the specifications on the various mirrors. The only significant change in foreoptics mirrors was to make M2 on a quartz blank. This was done because of its close proximity to the rod source and the small thermal expansion coefficient of quartz. The foreoptics mirrors are versatile enough to permit the use of a shorter 36.7 cm cell; however, the homogeneity of the field of the present Magion solenoid is sufficient to obviate its use.

The alignment procedure has been previously given (22). This has been facilitated by an assembly which positions a 25 watt Zr arc at the same point as the "carbon" rod.

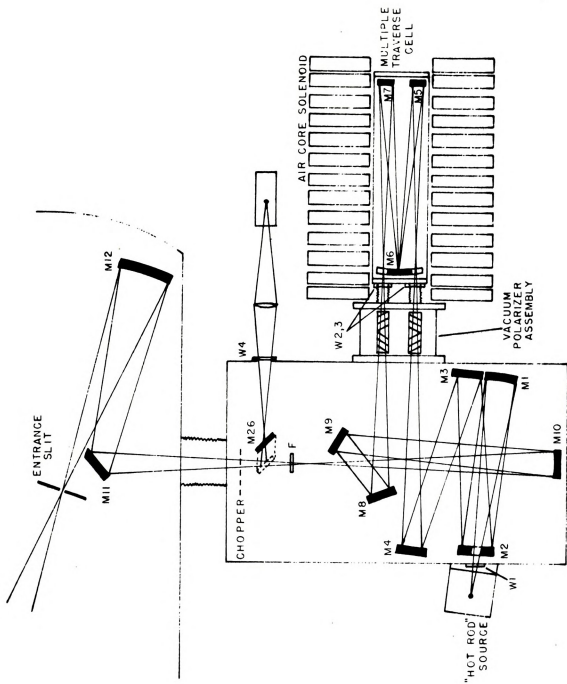


Fig. 8.3. Foreoptics, Polarizer Assembly and Solenoid.



Table 8.1 Spectrometer Optics

Element	Type	Comments
<u>Foreoptics</u>		
M1*	ellipse	4" dia; foci 44:176 cm
M2*	flat	3½" square; hole 2 cm dia. (fused silica blank)
M3,4*	flat	3½" square
M5,6,7*	sphere	6" dia., cut to make M5,6,7; R = 78.7 cm
M8,9*	flat	3½" square
M10*	ellipse	4" dia.; foci 128:64 cm
M11*	flat	4" square with beveled edge
M12*	ellipse	6" dia.; foci 114:57 cm
M26	flat	2" dia.
W1,2,3,4	window	CaF ₂ , 2", 1", 1", and 2" dia.
<u>Monochromator</u>		
M13*	parabola	10" dia.; focus 106 cm
M14	flat	10" dia.; rectangular hole 2.5 x 6 cm (cut off 10 cm from and parallel to hole)
M15	flat	10" dia.
G	grating	see text
M16	flat	4 x 3.4 cm, rear mount
<u>Exit Optics</u>		
M17*	ellipse	4" dia.; foci 40:112 cm
M18*	flat	4" dia.; hole 1.6 cm dia.
M19,20*	flat	2½" square
L1	plano-convex lens	2" dia.; foci -28:10; CaF ₂



Table 8.1 (cont.)

Element	Type	Comment
<u>Calibration Optics</u>		
W5,6	window	2" diameter
L2,3,4,5	convex lens	f = 25 cm; achromatic
M21,22,23	flat	2" x 2½"; 2 - ½" x ¾"
M24,25	flat	2" x 2½"
P	prism	height 2", long side 9.55 cm angles 50°, 60° and 70°

* Protected with SiO₂ coating

All mirrors are front surface type

The vacuum polarizer assembly is pictured in Fig. 8.4. It has provision for simultaneously removing both polarizer and analyzer from the beam to allow normal absorption or longitudinal Zeeman spectra to be recorded. In addition the polarizer and analyzer may be independently rotated and their angles readout to 0.1 degrees. This rotation is consistent with the conventions chosen in the MRS work. Two sets of polarizers will soon be available. The presently available set which operates between 2.5 and 12μ consists of 6 AgCl plates at Brewster's angle. The plates are mounted in precisely machined grooves in a tubelike structure made from "phenolboard." Equal numbers of plates are inclined in opposite directions to eliminate beam displacement upon rotation of the polarizer. This arrangement gives ~95 percent polarization. An Irtran II window is mounted in front of the first polarizer to eliminate the large amount of ultraviolet radiation which fogs the AgCl plates. The new set will use Polaroid HR plates as the polarizing elements and will be useful between 0.7 and 2.3μ .

F in Fig. 8.3 represents a filter holder by means of which one can insert any one of three IR filters for eliminating unwanted wavelengths from the beam. These filters cut off radiation below 1.06μ , 1.8μ and 3.0μ respectively.

Monochromator

Fig. 8.5 shows the present configuration of the monochromator. Modifications made here include: new entrance

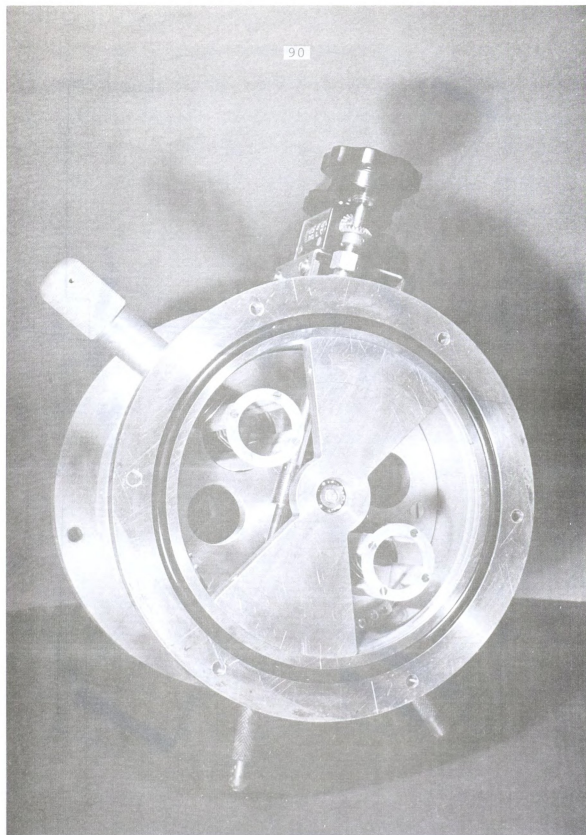


Fig. 8.4. Polarizer Assembly.



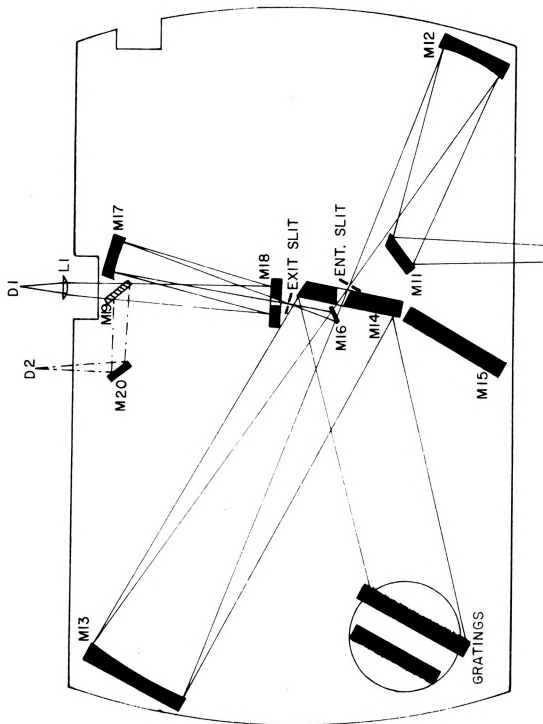


Fig. 8.5. Monochromator and Exit Optics.

slit jaws; insertion of two new 25 cm flats; a new pickoff mirror assembly; a new grating drive; and relocation of the gratings. As one might expect the entire monochromator had to be realigned and with insignificant exceptions the procedure given in (22) was followed.

The entrance slit is presently being formed by two razor blades manufactured by Edward Weck & Company. Almost every brand of razor blade currently manufactured was checked with a 30X microscope against the surface of a Johansen block. All blades with the exception of the Weck were found to have curvature and/or nicks in excess of 10μ . The Weck blades appear straight to within 1 or 2 microns over a length in excess of 2 cm and are free from nicks. These blades are mounted to the former slit jaws which have now been provided with an adjustable stop to prevent damaging the blades upon closing.

The greatest problem with this arrangement is in getting the two blades mounted in the same plane. The procedure used to accomplish this was to illuminate the slits from behind. The blades were then shimmed until no parallax existed as ones head was moved symmetrically from side to side. This procedure had to be carried out simultaneously with checking the blades for parallelism with the 30X microscope.

The flats M14 and M15, were identical 25 cm diameter mirrors and replace the former 20 cm diameter flats. This change allows the grating to be covered completely over a larger angular region and improves resolution at lower

angles. M14 has a rectangular hole 25 x 60 mm in its center and has been cut off along a line 10 cm from the center and parallel to the long axis of this hole. This allows a) the beam to enter the monochromator almost along the axis of the paraboloid and b) the exit slit to be placed as close to the pickoff mirror, M16, as possible. This latter feature allows the pickoff mirror to be as small as possible thus minimizing the amount of the beam obstructed. M15 is used for double passing the grating. To accomplish this M15 is rotated about a line perpendicular to the base plate and parallel to its face, to the best compromise position for covering the grating at working angles. It is then tipped until the double pass image at the exit slit is just below the single pass image. The pickoff mirror is tipped until the D.P. beam emerges from the exit slit parallel to the baseplate. The exit optics usually have to be realigned. The Foucault test must be repeated on the double pass image. Finally a mask should be placed at the exit slit to block out the single pass energy. Originally both modes of operation were to be simultaneously possible; however, the present hole in M18 is not sufficiently large to transmit both beams.

The grating equation for double pass is obtained as follows. The general grating equation is (71):

$$d(\sin i + \sin \theta) = m\lambda \quad , \quad (8.1)$$

where d is the grating space, i is the angle of incidence, θ is the angle of diffraction, m is the order, and λ is the

wavelength. θ is considered positive (negative) if it lies on the same (opposite) side of the normal as i . If ϕ is the angle between M14 and M15 measured from the axis of rotation of the grating, then for double pass, $\theta = i - \phi$; from which the equation can be written:

$$d[\sin i (1 + \cos 2f) - \sin 2f \cos i] = m\lambda \quad (8.2)$$

where $f = \phi/2$ is the angle of the double pass central image.

The new pickoff mirror assembly is merely a small stage which protrudes from the hole in M14 and provides a means of focusing, tipping and turning M16. This stage is fastened to the back of the mount for M14. This assembly eliminates all previous mounting arms which removed portions of the beam.

G is a mount which holds two Bausch & Lomb gratings mounted back to back. It has been repositioned so as to eliminate the so-called "single-double pass" radiation. This is radiation diffracted by the grating along the normal to the flat, so as to hit the flat, and then be reflected back to the grating to be dispersed again. There are three gratings available; a) 600 lines/mm with a ruled area of $212 \times 158 \text{ mm}^2$ blazed at 28.8° or 1.6μ in first order, b) 400 lines/mm with a ruled area of $206 \times 128 \text{ mm}^2$ blazed at 37.9° or 3μ in first order, and c) 300 lines/mm with a ruled area of $254 \times 128 \text{ mm}^2$ and blazed at 48.6° or 5μ in first order. Presently the 300 and 600 lines/mm gratings are mounted and the 300 lines/mm grating was used in this work.

Frequencies are measured on this instrument by a linear interpolation between calibrated interference fringes (53). Any variations in a uniform rotation of the grating will introduce uncertainties in the frequency of a line, a measure of which is the standard deviation of the calibration fit. A new grating drive train shown in Fig. 8.6, was installed to minimize and/or eliminate the variations which existed in the former selsyn drive system. Three things were done in this new system; a) the 14" bronze and companion screw gear of the 360:1 reducer were lapped against one another with fine grinding compound to make as smooth a contact as possible at this very critical point, b) all gears at the next critical point in the train were replaced by precision 3 gears, (PIC Design Corporation) having a maximum tooth to tooth uncertainty of 0.0001", c) the drive was made direct by means of an SR-37 Consolidated Vacuum Corporation double O-ring seal. These changes and other minor ones now enable the reproduction of the standard frequencies (53) with an average standard deviation of $\sim 0.002 \text{ cm}^{-1}$. The 10 speed variable reductor (Inesco Corporation) in the drive train gives shaft speeds of 0.01, 0.02, 0.05, 0.1, 0.2, 0.5, 1, 2, 5 and 10 RPM at the output of the 90:1 reducer. This in turn drives the grating the same number of degrees/minute. Spectra are normally recorded at 0.02, 0.05, or 0.1 degrees/minute.



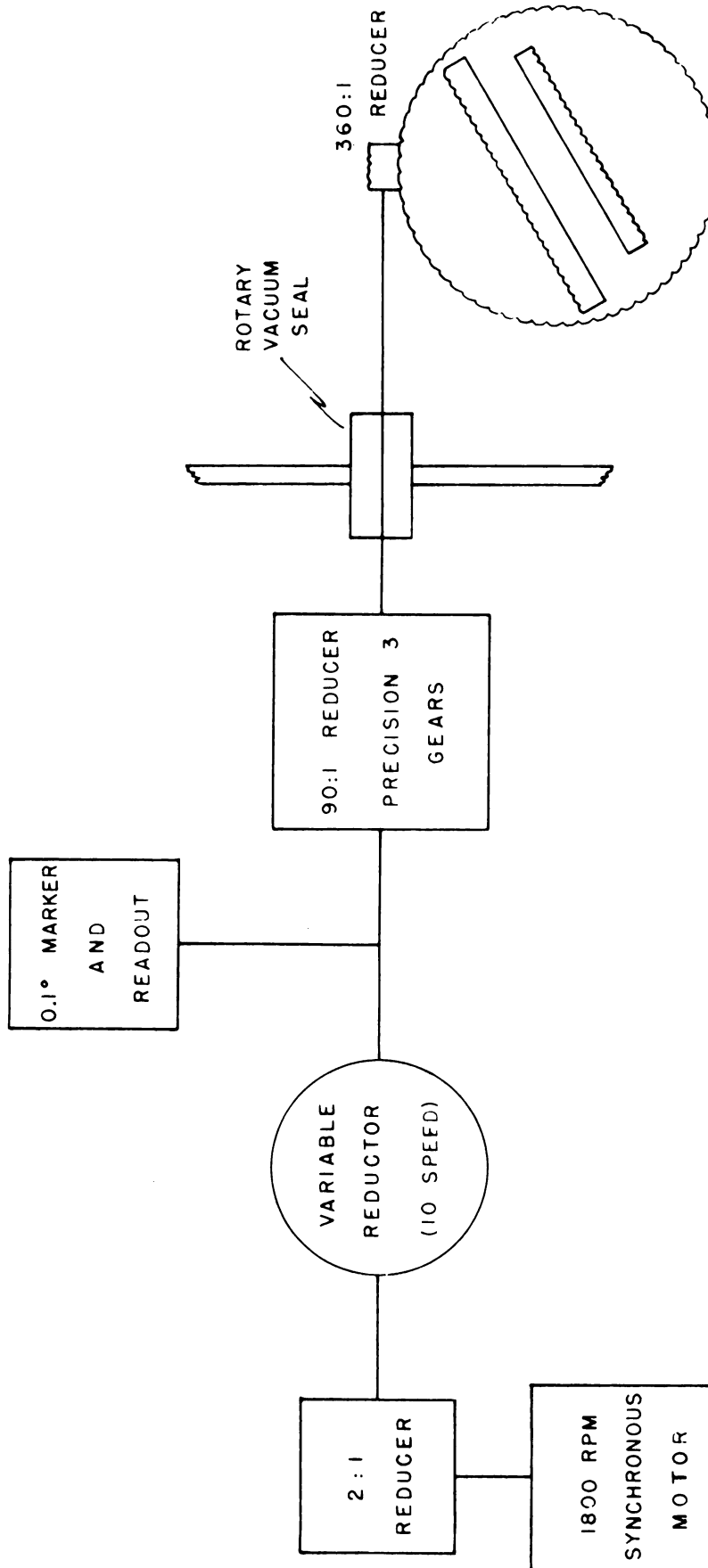


Fig. 8.6. Grating Drive Train



Fringe System

The present Edser-Butler calibration train is shown in Fig. 8.7. The major alteration here is the use of a constant deviation Wadsworth (72) assembly for order sorting which replaces the interference filters formerly used. This system was designed primarily by Dr. M. D. Olman.

The source for the calibration system is a 100 watt Zr arc. The chopper is driven by an 1800 RPM synchronous motor and interrupts the beam 450 times/sec. L2 and L3 deliver an f/5 beam to the monochromator by means of two front surface mirrors, M21 and M22. The fringe beam enters and leaves the monochromator symmetrically 2.1 cm above and below the axis of the paraboloid and traces basically the same path as the infrared beam. M23 directs the beam to a collimating lens, L4. The beam then passes through a Fabry-Perot etalon which has a spacing of 3.1102 ± 0.0003 mm.

The normal ring system is formed for each wavelength present in the beam. The condition for a maximum in transmission at the wavelength λ is (73):

$$2t \cos \phi = n\lambda \quad (8.3)$$

where ϕ is the angle between the axis and the n^{th} bright ring and t is the etalon spacing. If n is changed by unity this corresponds to a change:

$$\Delta \nu (\text{cm}^{-1}) = \frac{1}{2t} \quad (8.4)$$

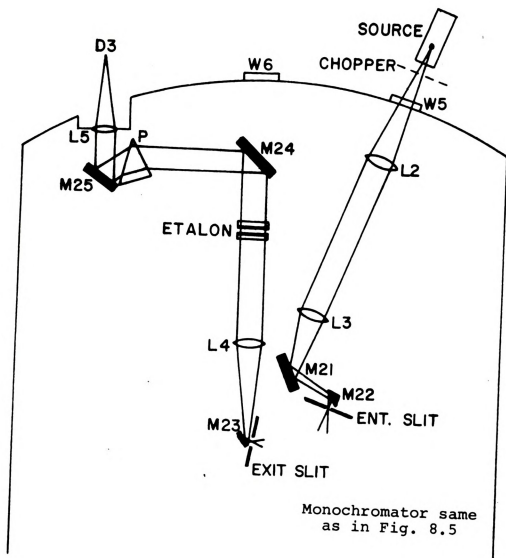


Fig. 8.7. Calibration System.

I
C
b
Il
on
wo.
vit
Tri

8888

at the angle $\phi = 0$. From the grating equation, the angle by which the grating must rotate to produce a change in n of one at the center of the pattern is found:

$$\Delta\theta = (2d \sin\theta \tan\theta) \left(\frac{1}{2\epsilon m} \right) \quad (8.5)$$

where d is the grating space, θ the grating angle and m the order of interference in the light coming from the grating. From this the relation between the change in v in the orders m and m' is:

$$\Delta v_{m'} = \frac{m'}{m} \Delta v_m = \frac{m'}{m} \frac{1}{2\epsilon} \quad (8.6)$$

M24 directs the beam to a prism in a Wadsworth mount which acts as an order sorter. The order sorter must be placed in the exit optics system so that the same light distribution is maintained in the monochromator at all times. The prism is mounted at minimum deviation and the combination of the prism and M25 form a constant deviation device. L5 brings the various orders to focus in the plane D3. A 1P21 photomultiplier with a slit taped on its face is placed on the axis of L5. By adjustment of a feed screw the Wadsworth assembly brings one of the orders into coincidence with this slit.

Fringe System Alignment

Since the fringe system uses the monochromator, it is assumed that part of the alignment is already done.



at the angle $\phi = 0$. From the grating equation, the angle by which the grating must rotate to produce a change in n of one at the center of the pattern is found:

$$\Delta\theta = (2d \sin\theta \tan\theta) \left(\frac{1}{2\tau m} \right) \quad (8.5)$$

where d is the grating space, θ the grating angle and m the order of interference in the light coming from the grating. From this the relation between the change in v in the orders m and m' is:

$$\Delta v_{m'} = \frac{m'}{m} \Delta v_m = \frac{m'}{m} \frac{1}{2\tau} \quad (8.6)$$

M24 directs the beam to a prism in a Wadsworth mount which acts as an order sorter. The order sorter must be placed in the exit optics system so that the same light distribution is maintained in the monochromator at all times. The prism is mounted at minimum deviation and the combination of the prism and M25 form a constant deviation device. L5 brings the various orders to focus in the plane D3. A 1P21 photomultiplier with a slit taped on its face is placed on the axis of L5. By adjustment of a feed screw the Wadsworth assembly brings one of the orders into coincidence with this slit.

Fringe System Alignment

Since the fringe system uses the monochromator, it is assumed that part of the alignment is already done.

1. Position source and chopper on the axis of L2 and L3.
2. Position L2 so that the "bead" of the source is at its focal point. This may be done by observing the beam after L2 with a collimated telescope and adjusting L2 for the best image.
3. L3, M21, and M22 must be simultaneously adjusted to give a sharp image of the source on the entrance slit 17.2 cm above the baseplate and to cover the paraboloid symmetrically. With this done the beam will automatically leave the monochromator 0.9 cm below the IR beam. M23 is now tipped and/or turned to give uniform coverage on L4. L4 should be adjusted so that the beam travels along its axis.
4. With a collimated telescope, observe the beam leaving L4 and adjust L4 for the best image of the exit slit. A collimated beam is now leaving L4.
5. Insert M24 so that it intercepts the total beam and directs it to cover the face of the prism uniformly.
6. Remove M25 and adjust the prism for minimum deviation with the feed screw.
7. Insert M25 and adjust it until the beam travels along the axis of and uniformly covers L5. Lock down M25.
8. Connect the external drive and counter to the feed screw.
9. Insert the photomultiplier so that its slit is on the axis of L5 and the image of the exit slit is in focus on it.

10. Insert the etalon. Place a sodium lamp in the vicinity of L4 and observe output from the etalon with a telescope through W6 by removing M24. A ring pattern and image of the exit slit should be simultaneously visible. Adjust the etalon horizontally and vertically until the slit image is exactly centered in the ring pattern. The exit slit image is considerably smaller than the central spot in the ring pattern in order that good modulation is obtained. In this step it is assumed that the etalon plates are perfectly parallel by a previous adjustment.
11. Repeat Step 5 by using central image for sufficient intensity.

This completes alignment and the entire train must now be carefully shielded to prevent stray light from reaching the photomultiplier.

Detectors

A number of new detectors have been obtained. These include Kodak types N-2, O-2, P-2 and E-2. The N-2, O-2 and P-2 are PbS cells while the E-2 is a PbSe cell. All are coolable.

The PbSe E-2 detector has a sensitive area of 0.2×4 mm and is most useful from $\sim 4.25\mu - 6.5\mu$. It was used for this work. It has a room temperature resistance of $\sim 2300\Omega$, a 77°K resistance of $\sim 8\text{M}\Omega$, and needs a 9V bias battery. Be-
cause of its sensitivity at comparatively long wavelengths

the use of a cooled light shield which allows only radiation from the monochromator to strike it is absolutely essential. Without this shield it was found that the detectivity can be reduced by as much as a factor of 10. The linearity of the PbSe E-2 detector has not been checked. This must be done before quantitative intensity measurements are made.

These detectors are, or soon will be, mounted on a brass base by means of Dow Corning "Silastic". The brass base is recommended by Kodak to match the thermal expansion coefficient of the detector.

Electronics

With the exception of the infrared preamplifier the electronics is as described by Aubel (22). The preamp presently in use is a battery operated solid state FET device obtained from Denro Labs. It has a frequency response flat within 2 db from 8 to 10^5 cps, a continuously variable voltage gain of from 10-100 times that input, and an input impedance in excess of 140 M Ω . It has been found that the noise equivalent signal (i.e., that signal necessary to produce an SNR of unity) of this solid state device is essentially the same as the formerly used Tektronix Model 122 preamp, and requires three fewer power supplies.

Recommendations

During the course of work on this instrument, it was noted that a number of other changes could be made which would potentially improve its operation.

New entrance and exit slit mounts and drives should be constructed. Presently these mechanisms do not even have the same pitch drive screw. Provision for more accurate setting and readout of the slit opening should be made.

A new detector housing should be constructed. It should have provision for mounting several detectors with a means of quickly changing them without first warming them. An adjustable and coolable light shield should be provided. The detectors are presently the limiting noise factor. Some evidence exists for obtaining improved detectivity by adjusting the detector temperature for a given wavelength. It appears that with the use of a small heater coil, the temperature of a detector could be adjusted to and held at any temperature from 77°K to room temperature. Further tests should be run on this with the detectors and incorporated in any new housing if the improvement warrants it. Some improvement might also be obtained by selecting the optimum chopping frequency, this however requires major modifications.

SUMMARY

An analysis of the vibration-rotation transitions for the 1-0 band including lines from the HES and LES for both $^{14}\text{N}^{16}\text{O}$ and $^{15}\text{N}^{16}\text{O}$ has been performed. Least squares fits of both combination differences and frequencies has led to improved values of the rotational, vibrational and spin-orbit constants. Values for the λ -doubling constants have also been obtained. Isotopic substitution calculations were carried out and agree well with observation.

Zeeman patterns were resolved for the lowest J-values of the fundamental band and the splittings agree reasonably well with theory.

The magnetic rotation spectra of the fundamental band for the above two isotopes was recorded. Quantum mechanical calculation of Zeeman intensities, inserted into a classically derived expression, and inclusion of the effects of a finite resolution spectrometer has led to predictions for the magnetic rotation spectra which agree with the major features of the observed spectra. These predictions have led to greater understanding of the magnetic rotation effect.

Modifications were made on the high resolution infrared spectrometer which have increased its range, and improved its accuracy and ease of operation. These included addition of a rod source, a vacuum polarizer assembly and a new grating drive assembly.



REFERENCES

1. R. H. Gillete and E. H. Eyster, Phys. Rev. 56, 1113 (1939).
2. C. A. Burrus and W. Gordy, Phys. Rev. 92, 1437 (1953).
3. J. J. Gallagher, F. D. Bedard and C. M. Johnson, Phys. Rev. 93, 729 (1954).
4. N. L. Nichols, C. D. Hause and R. H. Noble, J. Chem. Phys. 23, 57 (1955).
5. J. J. Gallagher and C. M. Johnson, Phys. Rev. 103, 1727 (1956).
6. J. H. Shaw, J. Chem. Phys. 24, 399 (1956).
7. E. D. Palik and K. N. Rao, J. Chem. Phys. 25, 1174 (1956).
8. W. H. Fletcher and G. M. Begun, J. Chem. Phys. 27, 579 (1957).
9. P. G. Favero, A. M. Mirri and W. Gordy, Phys. Rev. 114, 1534 (1959).
10. Ph. Arcas, C. Haeusler, C. Joffrin, C. Meyer, Nguyen Van Thanh, and P. Barchewitz, Appl. Optics, 2, 909 (1953).
11. M. D. Olman, M. D. McNelis and C. D. Hause, J. Mol. Spectry. 14, 62 (1964).
12. T. C. James, J. Chem. Phys. 40, 762 (1964).
13. T. C. James and R. J. Thibault, J. Chem. Phys. 41, 2806 (1964).
14. C. Meyer, C. Haeusler, and P. Barchewitz, J. de Physique, 26, 799 (1965).
15. J. F. Watkins and J. H. Shaw, paper C3, Ohio State University Symposium on Molecular Structure and Spectroscopy, (1966).
16. J. L. Griggs, K. N. Rao, L. H. Jones and R. M. Potter, J. Mol. Spectry. 22, 383 (1967).

17. E. Hill and J. H. Van Vleck, *Phys. Rev.* 32, 250 (1928).
18. J. H. Van Vleck, *Phys. Rev.* 33, 467 (1929).
19. G. M. Almy and R. B. Horsfall, Jr., *Phys. Rev.* 51, 441 (1937).
20. G. C. Dousmanis, T. M. Sanders, and C. H. Townes, *Phys. Rev.* 100, 1735 (1955).
21. A. D. Buckingham and P. J. Stephens, "Magnetic Optical Activity", *Annual Review of Physical Chemistry*, Vol. 17. (Annual Reviews, Inc., Palo Alto, California, 1966). pp. 399-432.
22. J. L. Aubel, Thesis, Michigan State University (1964).
23. G. Herzberg, *Spectra of Diatomic Molecules*, p. 149, 2nd Ed., D. Van Nostrand, New York (1950).
24. Ibid., p. 92.
25. Ibid., pp. 218-226.
26. R. de L. Kronig, *Z. Physik*, 46, 814; 50, 347 (1928).
27. R. S. Mulliken, *Rev. Mod. Phys.* 3, 89 (1931).
28. L. Pauling and E. Bright Wilson, *Introduction to Quantum Mechanics*, pp. 271-274, McGraw-Hill, New York (1935).
29. Herzberg, *op. cit.* pp. 226-229, 268-271.
30. W. Gordy, W. V. Smith and R. F. Trambarulo, *Microwave Spectroscopy*, pp. 185-188, John Wiley and Sons, New York (1953).
31. C. H. Townes and A. L. Schawlow, *Microwave Spectroscopy*, pp. 343-344, McGraw-Hill, New York (1955).
32. Pauling and Wilson, *op. cit.*, pp. 302-306.
33. Herzberg, *op. cit.*, p. 94.
34. P. C. Cross, R. M. Hainer, and G. W. King, *J. Chem. Phys.* 12, 210 (1944).
35. Herzberg, *op. cit.*, p. 241.
36. Townes and Schawlow, *op. cit.*, pp. 19-20.

37. J. R. Izatt, Self and Foreign Gas Broadening in the Pure Rotation Spectrum of Water Vapor, p. 34, Progress Report, The John Hopkins University Laboratory of Astrophysics and Physical Meteorology, Baltimore 18, Maryland. (1960).
38. L. L. Abels and J. H. Shaw, J. Mol. Spectry. 20, 11 (1966).
39. C. C. Lin, Thesis, Harvard University (1955).
40. L. I. Schiff, Quantum Mechanics, pp. 150-152, 1st Ed., McGraw-Hill, New York. (1949).
41. M. Faraday, Phil. Mag., 28, 294 (1846); Phil. Trans. Roy. Soc. London (1846)
42. L. Rosenfeld, Z. Physik, 57, 835 (1929).
43. H. A. Kramers, Proc. Acad. Sci., Amsterdam, 33, 959 (1930).
44. R. Serber, Phys. Rev., 41, 489 (1932).
45. T. Carroll, Phys. Rev. 52, 822 (1937).
46. H. F. Hameka, J. Chem. Phys. 36, 2540 (1962).
47. H. F. Hameka, J. Chem. Phys. 37, 2209 (1962).
48. D. F. Hutchenson and H. F. Hameka, J. Mol. Spectry. 18, 141 (1965).
49. S. S. Penner, Quantitative Molecular Spectroscopy and Gas Emissivities, Chaps. 3 and 4, Addison Wesley, Reading, Mass. (1959).
50. Izatt, op. cit., p. 37.
51. C. Kittel, Elementary Statistical Physics, pp. 206-210, John Wiley, New York. (1958)
52. E. U. Condon and G. H. Shortley, The Theory of Atomic Spectra, p. 379, MacMillan, Cambridge, England (1935).
53. K. N. Rao, C. J. Humphreys and D. H. Rank, Wavelength Standards in the Infrared, pp. 160-162, 171, Academic Press, New York. (1966).
54. This system, originally used to digitize cloud chamber data, was recognized to be applicable to the reduction of spectroscopic data by Prof. T. H. Edwards. Line position measurements can be reproduced to better than

0.03 mm on the original charts and the X-Y coordinates punched out on computer cards. The system is described briefly by T. L. Barnett, Thesis, Michigan State University (1967) and T. H. Edwards, J. Opt. Soc. Am. 52, 1311 (1962).

55. Herzberg, op. cit., pp. 175-185.
56. J. W. Boyd, Thesis, Michigan State University (1963). H. Scheffe, The Analysis of Variance, Chap. 3, Wiley, New York (1959). The SCI means that, for a level of significance α , there is a probability of $(1-\alpha)$ that all estimators for the constants will simultaneously be within their SCI of the "true" value of the constants.
57. American Institute of Physics Handbook, pp. 8-6, McGraw-Hill, New York, (1967).
58. Herzberg, op. cit., p. 175.
59. R. Beringer, E. B. Rawson, and A. F. Henry, Phys. Rev. 94, 343 (1954).
60. M. Mizushima, J. T. Cox and W. Gordy, Phys. Rev. 98, 1034 (1955).
61. R. L. Brown and H. E. Radford, Phys. Rev. 147, 6 (1966).
62. G. A. Mann and C. D. Hause, J. Chem. Phys. 33, 1117 (1960).
63. J. L. Aubel and C. D. Hause, J. Chem. Phys. 44, 2659 (1966).
64. D. W. Robinson, J. Chem. Phys. 46, 4525 (1967).
65. A. D. Buckingham and G. A. Segal, Private communication.
66. A. F. Stalder and W. H. Eberhardt, Private communication.
67. R. H. Noble, J. Opt. Soc. Am. 43, 330 (1953).
68. R. G. Brown, Theses, Michigan State University (1957, 1959).
69. D. H. Rank, Private communication.
70. R. Spanbauer, P. E. Fraley and K. N. Rao, Appl. Opt. 2, 1340 (1963).
71. F. A. Jenkins and H. E. White, Fundamentals of Optics, p. 333, 3rd Ed., McGraw-Hill, New York (1957).
72. F. O. L. Wadsworth, Astrophys. 1, 232 (1895); 2, 264 (1895).
73. Jenkins and White, op. cit., p. 275.

- 74. M. D. Olman, Thesis, Michigan State University (1967).
- 75. M. A. Efroymsen, Mathematical Methods for Digital Computers, Chap. 17, John Wiley, New York. (1960).



APPENDIX I

Assume the following phase convention:

$$\langle \Omega | J_Y | \Omega \pm 1 \rangle = i \langle \Omega | J_X | \Omega \pm 1 \rangle = F(J)$$

$$-\langle \Sigma | S_Y | \Sigma \pm 1 \rangle = i \langle \Sigma | S_X | \Sigma \pm 1 \rangle = F(S)$$

$$-\langle \Lambda | L_Y | \Lambda \pm 1 \rangle = i \langle \Lambda | L_X | \Lambda \pm 1 \rangle$$

where

$$F(X) = \frac{1}{2} [X(X+1) - X_Z(X_Z \pm 1)]^{\frac{1}{2}}$$

A) Matrix Elements of H'_r .

$$\langle \Sigma_{\frac{1}{2}} | H'_r | \Sigma_{\frac{1}{2}} \rangle = \langle \Sigma_{-\frac{1}{2}} | H'_r | \Sigma_{-\frac{1}{2}} \rangle = B^{\sigma} [J(J+1) + \frac{1}{4}] + E \equiv \alpha$$

$$\begin{aligned} \langle \Pi_{\frac{1}{2}} | H'_r | \Pi_{\frac{1}{2}} \rangle &= \langle \Pi_{-\frac{1}{2}} | H'_r | \Pi_{-\frac{1}{2}} \rangle = B^{\pi} \{ [J(J+1) + \frac{1}{4}] \\ &\quad + [L(L+1) - \Lambda^2] \} \equiv \beta_1 \end{aligned}$$

$$\begin{aligned} \langle \Pi_{\frac{3}{2}} | H'_r | \Pi_{\frac{3}{2}} \rangle &= \langle \Pi_{-\frac{3}{2}} | H'_r | \Pi_{-\frac{3}{2}} \rangle = B^{\pi} \{ [J(J+1) - \frac{7}{4}] \\ &\quad + [L(L+1) - \Lambda^2] \} \equiv \gamma_1 \end{aligned}$$

$$\langle \Sigma_{\frac{1}{2}} | H'_r | \Sigma_{-\frac{1}{2}} \rangle = B^{\sigma} (J + \frac{1}{2}) \equiv \delta$$

$$\langle \Pi_{\frac{3}{2}} | H'_r | \Pi_{\frac{1}{2}} \rangle = \langle \Pi_{-\frac{3}{2}} | H'_r | \Pi_{-\frac{1}{2}} \rangle = B^{\pi} [(J - \frac{1}{2}) (J + \frac{3}{2})]^{\frac{1}{2}} \equiv \epsilon$$

$$\langle \Pi_{\frac{1}{2}} | H'_r | \Sigma_{-\frac{1}{2}} \rangle = \langle \Pi_{-\frac{1}{2}} | H'_r | \Sigma_{\frac{1}{2}} \rangle = -2 \langle \Pi | BL_Y | \Sigma \rangle (J + \frac{1}{2}) \equiv \zeta$$

$$\begin{aligned} \langle \Pi_{\frac{3}{2}} | H'_r | \Sigma_{\frac{1}{2}} \rangle &= \langle \Pi_{-\frac{3}{2}} | H'_r | \Sigma_{-\frac{1}{2}} \rangle = -2 \langle \Pi | BL_Y | \Sigma \rangle \times \\ &\quad [(J - \frac{1}{2}) (J + \frac{3}{2})]^{\frac{1}{2}} \equiv \eta \end{aligned}$$

$$\langle \Pi_{\frac{1}{2}} | H'_r | \Sigma_{\frac{1}{2}} \rangle = \langle \Pi_{-\frac{1}{2}} | H'_r | \Sigma_{-\frac{1}{2}} \rangle = -2 \langle \Pi | BL_Y | \Sigma \rangle \equiv \theta_1$$

APPENDIX I

Assume the following phase convention:

$$\langle \Omega | J_Y | \Omega \pm 1 \rangle = i \langle \Omega | J_X | \Omega \pm 1 \rangle = F(J)$$

$$-\langle \Sigma | S_Y | \Sigma \pm 1 \rangle = i \langle \Sigma | S_X | \Sigma \pm 1 \rangle = F(S)$$

$$-\langle \Lambda | L_Y | \Lambda \pm 1 \rangle = i \langle \Lambda | L_X | \Lambda \pm 1 \rangle$$

where $F(X) = \frac{1}{2} [X(X+1) - X_Z(X_Z \pm 1)]^{\frac{1}{2}}$

A) Matrix Elements of H'_r .

$$\langle \Sigma_{\frac{1}{2}} | H'_r | \Sigma_{\frac{1}{2}} \rangle = \langle \Sigma_{-\frac{1}{2}} | H'_r | \Sigma_{-\frac{1}{2}} \rangle = B^\sigma [J(J+1) + \frac{1}{4}] + E \equiv \alpha$$

$$\begin{aligned} \langle \Pi_{\frac{1}{2}} | H'_r | \Pi_{\frac{1}{2}} \rangle &= \langle \Pi_{-\frac{1}{2}} | H'_r | \Pi_{-\frac{1}{2}} \rangle = B^\pi \{ [J(J+1) + \frac{1}{4}] \\ &\quad + [L(L+1) - \Lambda^2] \} \equiv \beta_1 \end{aligned}$$

$$\begin{aligned} \langle \Pi_{\frac{3}{2}} | H'_r | \Pi_{\frac{3}{2}} \rangle &= \langle \Pi_{-\frac{3}{2}} | H'_r | \Pi_{-\frac{3}{2}} \rangle = B^\pi \{ [J(J+1) - \frac{7}{4}] \\ &\quad + [L(L+1) - \Lambda^2] \} \equiv \gamma_1 \end{aligned}$$

$$\langle \Sigma_{\frac{1}{2}} | H'_r | \Sigma_{-\frac{1}{2}} \rangle = B^\sigma (J + \frac{1}{2}) \equiv \delta$$

$$\langle \Pi_{\frac{3}{2}} | H'_r | \Pi_{\frac{1}{2}} \rangle = \langle \Pi_{-\frac{3}{2}} | H'_r | \Pi_{-\frac{1}{2}} \rangle = B^\pi [(J - \frac{1}{2})(J + \frac{3}{2})]^{\frac{1}{2}} \equiv \epsilon$$

$$\langle \Pi_{\frac{1}{2}} | H'_r | \Sigma_{-\frac{1}{2}} \rangle = \langle \Pi_{-\frac{1}{2}} | H'_r | \Sigma_{\frac{1}{2}} \rangle = -2 \langle \Pi | BL_Y | \Sigma \rangle (J + \frac{1}{2}) \equiv \zeta$$

$$\begin{aligned} \langle \Pi_{\frac{3}{2}} | H'_r | \Sigma_{\frac{1}{2}} \rangle &= \langle \Pi_{-\frac{3}{2}} | H'_r | \Sigma_{-\frac{1}{2}} \rangle = -2 \langle \Pi | BL_Y | \Sigma \rangle \times \\ &\quad [(J - \frac{1}{2})(J + \frac{3}{2})]^{\frac{1}{2}} \equiv \eta \end{aligned}$$

$$\langle \Pi_{\frac{1}{2}} | H'_r | \Sigma_{\frac{1}{2}} \rangle = \langle \Pi_{-\frac{1}{2}} | H'_r | \Sigma_{-\frac{1}{2}} \rangle = -2 \langle \Pi | BL_Y | \Sigma \rangle \equiv \theta_1$$



Note: The phase conventions chosen are not those of VanVleck (15) or Dousmanis, Sanders and Townes (20). They are chosen in such a way as to agree with those of King, Hainer and Cross (34) used in calculating the direction cosine matrix elements and yet yield the energies as derived by VanVleck. The constant term $L^2 - \Lambda^2$ has been included.

B) Matrix Elements of $A(\vec{L} \cdot \vec{S})$.

$$\langle \Pi_{-\frac{3}{2}} | A(\vec{L} \cdot \vec{S}) | \Pi_{-\frac{3}{2}} \rangle = \langle \Pi_{\frac{3}{2}} | A(\vec{L} \cdot \vec{S}) | \Pi_{\frac{3}{2}} \rangle = \frac{1}{2}A = \gamma_2$$

$$\langle \Pi_{-\frac{1}{2}} | A(\vec{L} \cdot \vec{S}) | \Pi_{-\frac{1}{2}} \rangle = \langle \Pi_{\frac{1}{2}} | A(\vec{L} \cdot \vec{S}) | \Pi_{\frac{1}{2}} \rangle = -\frac{1}{2}A = \beta_2$$

$$\langle \Pi_{\frac{1}{2}} | A(\vec{L} \cdot \vec{S}) | \Sigma_{\frac{1}{2}} \rangle = \langle \Pi_{-\frac{1}{2}} | A(\vec{L} \cdot \vec{S}) | \Sigma_{-\frac{1}{2}} \rangle = \langle \Pi | A L_Y | \Sigma \rangle = \theta_2$$

To simplify notation the following definitions are made:

$$\beta \equiv \beta_1 + \beta_2$$

$$\gamma \equiv \gamma_1 + \gamma_2$$

$$\theta \equiv \theta_1 + \theta_2$$

$$\kappa^{S,a} = \alpha \pm \delta$$

$$\mu^{S,a} = \theta \pm \zeta$$



APPENDIX II-A

INTERMEDIATE WAVE FUNCTIONS FOR THE
2 PI 1/2, v=0 STATE OF 14N16O AS A FUNCTION OF J

[S,J,M) = A		[J,M,S> - B		[J,M,S>	
[1/2, 1/2,M)	=1.000[1/2,M,1/2>	-0.000[1/2,M,3/2>			
[1/2, 3/2,M)	=1.000[3/2,M,1/2>	-0.024[3/2,M,3/2>			
[1/2, 5/2,M)	=0.999[5/2,M,1/2>	-0.040[5/2,M,3/2>			
[1/2, 7/2,M)	=0.999[7/2,M,1/2>	-0.054[7/2,M,3/2>			
[1/2, 9/2,M)	=0.998[9/2,M,1/2>	-0.069[9/2,M,3/2>			
[1/2,11/2,M)	=0.997[11/2,M,1/2>	-0.083[11/2,M,3/2>			
[1/2,13/2,M)	=0.995[13/2,M,1/2>	-0.096[13/2,M,3/2>			
[1/2,15/2,M)	=0.994[15/2,M,1/2>	-0.110[15/2,M,3/2>			
[1/2,17/2,M)	=0.992[17/2,M,1/2>	-0.123[17/2,M,3/2>			
[1/2,19/2,M)	=0.991[19/2,M,1/2>	-0.137[19/2,M,3/2>			
[1/2,21/2,M)	=0.989[21/2,M,1/2>	-0.149[21/2,M,3/2>			
[1/2,23/2,M)	=0.987[23/2,M,1/2>	-0.162[23/2,M,3/2>			
[1/2,25/2,M)	=0.985[25/2,M,1/2>	-0.175[25/2,M,3/2>			
[1/2,27/2,M)	=0.982[27/2,M,1/2>	-0.187[27/2,M,3/2>			
[1/2,29/2,M)	=0.980[29/2,M,1/2>	-0.199[29/2,M,3/2>			
[1/2,31/2,M)	=0.978[31/2,M,1/2>	-0.210[31/2,M,3/2>			
[1/2,33/2,M)	=0.975[33/2,M,1/2>	-0.222[33/2,M,3/2>			
[1/2,35/2,M)	=0.973[35/2,M,1/2>	-0.233[35/2,M,3/2>			
[1/2,37/2,M)	=0.970[37/2,M,1/2>	-0.244[37/2,M,3/2>			
[1/2,39/2,M)	=0.967[39/2,M,1/2>	-0.254[39/2,M,3/2>			
[1/2,41/2,M)	=0.964[41/2,M,1/2>	-0.264[41/2,M,3/2>			
[1/2,43/2,M)	=0.962[43/2,M,1/2>	-0.274[43/2,M,3/2>			
[1/2,45/2,M)	=0.959[45/2,M,1/2>	-0.284[45/2,M,3/2>			
[1/2,47/2,M)	=0.956[47/2,M,1/2>	-0.293[47/2,M,3/2>			
[1/2,49/2,M)	=0.953[49/2,M,1/2>	-0.302[49/2,M,3/2>			

INTERMEDIATE WAVE FUNCTIONS FOR THE
2 PI 3/2, v=0 STATE OF 14N16O AS A FUNCTION OF J

[S,J,M)	=	A	[J,M,S>	+	B	[J,M,S>
[3/2, 1/2,M)	=	1.000	[1/2,M,3/2>	+	0.000	[1/2,M,1/2>
[3/2, 3/2,M)	=	1.000	[3/2,M,3/2>	+	0.024	[3/2,M,1/2>
[3/2, 5/2,M)	=	0.999	[5/2,M,3/2>	+	0.040	[5/2,M,1/2>
[3/2, 7/2,M)	=	0.999	[7/2,M,3/2>	+	0.054	[7/2,M,1/2>
[3/2, 9/2,M)	=	0.998	[9/2,M,3/2>	+	0.069	[9/2,M,1/2>
[3/2,11/2,M)	=	0.997	[11/2,M,3/2>	+	0.083	[11/2,M,1/2>
[3/2,13/2,M)	=	0.995	[13/2,M,3/2>	+	0.096	[13/2,M,1/2>
[3/2,15/2,M)	=	0.994	[15/2,M,3/2>	+	0.110	[15/2,M,1/2>
[3/2,17/2,M)	=	0.992	[17/2,M,3/2>	+	0.123	[17/2,M,1/2>
[3/2,19/2,M)	=	0.991	[19/2,M,3/2>	+	0.137	[19/2,M,1/2>
[3/2,21/2,M)	=	0.989	[21/2,M,3/2>	+	0.149	[21/2,M,1/2>
[3/2,23/2,M)	=	0.987	[23/2,M,3/2>	+	0.162	[23/2,M,1/2>
[3/2,25/2,M)	=	0.985	[25/2,M,3/2>	+	0.175	[25/2,M,1/2>
[3/2,27/2,M)	=	0.982	[27/2,M,3/2>	+	0.187	[27/2,M,1/2>
[3/2,29/2,M)	=	0.980	[29/2,M,3/2>	+	0.199	[29/2,M,1/2>
[3/2,31/2,M)	=	0.978	[31/2,M,3/2>	+	0.210	[31/2,M,1/2>
[3/2,33/2,M)	=	0.975	[33/2,M,3/2>	+	0.222	[33/2,M,1/2>
[3/2,35/2,M)	=	0.973	[35/2,M,3/2>	+	0.233	[35/2,M,1/2>
[3/2,37/2,M)	=	0.970	[37/2,M,3/2>	+	0.244	[37/2,M,1/2>
[3/2,39/2,M)	=	0.967	[39/2,M,3/2>	+	0.254	[39/2,M,1/2>
[3/2,41/2,M)	=	0.964	[41/2,M,3/2>	+	0.264	[41/2,M,1/2>
[3/2,43/2,M)	=	0.962	[43/2,M,3/2>	+	0.274	[43/2,M,1/2>
[3/2,45/2,M)	=	0.959	[45/2,M,3/2>	+	0.284	[45/2,M,1/2>
[3/2,47/2,M)	=	0.956	[47/2,M,3/2>	+	0.293	[47/2,M,1/2>
[3/2,49/2,M)	=	0.953	[49/2,M,3/2>	+	0.302	[49/2,M,1/2>



INTERMEDIATE WAVE FUNCTIONS FOR THE
2 P₁ 1/2, v=1 STATE OF 14N16O AS A FUNCTION OF J

(S, L, M)	=	A	(J, M, S)	=	B	(J, M, S)
(1/2, 1/2, M)	=	1.000	(1/2, M, 1/2)	=	0.000	(1/2, M, 3/2)
(1/2, 3/2, M)	=	1.000	(3/2, M, 1/2)	=	-0.024	(3/2, M, 3/2)
(1/2, 5/2, M)	=	0.999	(5/2, M, 1/2)	=	-0.040	(5/2, M, 3/2)
(1/2, 7/2, M)	=	0.999	(7/2, M, 1/2)	=	-0.054	(7/2, M, 3/2)
(1/2, 9/2, M)	=	0.998	(9/2, M, 1/2)	=	-0.068	(9/2, M, 3/2)
(1/2, 11/2, M)	=	0.997	(11/2, M, 1/2)	=	-0.082	(11/2, M, 3/2)
(1/2, 13/2, M)	=	0.995	(13/2, M, 1/2)	=	-0.096	(13/2, M, 3/2)
(1/2, 15/2, M)	=	0.994	(15/2, M, 1/2)	=	-0.109	(15/2, M, 3/2)
(1/2, 17/2, M)	=	0.992	(17/2, M, 1/2)	=	-0.123	(17/2, M, 3/2)
(1/2, 19/2, M)	=	0.991	(19/2, M, 1/2)	=	-0.136	(19/2, M, 3/2)
(1/2, 21/2, M)	=	0.989	(21/2, M, 1/2)	=	-0.149	(21/2, M, 3/2)
(1/2, 23/2, M)	=	0.987	(23/2, M, 1/2)	=	-0.161	(23/2, M, 3/2)
(1/2, 25/2, M)	=	0.985	(25/2, M, 1/2)	=	-0.174	(25/2, M, 3/2)
(1/2, 27/2, M)	=	0.983	(27/2, M, 1/2)	=	-0.186	(27/2, M, 3/2)
(1/2, 29/2, M)	=	0.980	(29/2, M, 1/2)	=	-0.198	(29/2, M, 3/2)
(1/2, 31/2, M)	=	0.978	(31/2, M, 1/2)	=	-0.209	(31/2, M, 3/2)
(1/2, 33/2, M)	=	0.975	(33/2, M, 1/2)	=	-0.221	(33/2, M, 3/2)
(1/2, 35/2, M)	=	0.973	(35/2, M, 1/2)	=	-0.232	(35/2, M, 3/2)
(1/2, 37/2, M)	=	0.970	(37/2, M, 1/2)	=	-0.242	(37/2, M, 3/2)
(1/2, 39/2, M)	=	0.968	(39/2, M, 1/2)	=	-0.253	(39/2, M, 3/2)
(1/2, 41/2, M)	=	0.965	(41/2, M, 1/2)	=	-0.263	(41/2, M, 3/2)
(1/2, 43/2, M)	=	0.962	(43/2, M, 1/2)	=	-0.273	(43/2, M, 3/2)
(1/2, 45/2, M)	=	0.959	(45/2, M, 1/2)	=	-0.283	(45/2, M, 3/2)
(1/2, 47/2, M)	=	0.956	(47/2, M, 1/2)	=	-0.292	(47/2, M, 3/2)
(1/2, 49/2, M)	=	0.954	(49/2, M, 1/2)	=	-0.301	(49/2, M, 3/2)

INTERMEDIATE WAVE FUNCTIONS FOR THE
2 P1 3/2, V=1 STATE OF 14N16O AS A FUNCTION OF J

$$[S, J, M] = A [J, M, S] + B [J, M, S]$$

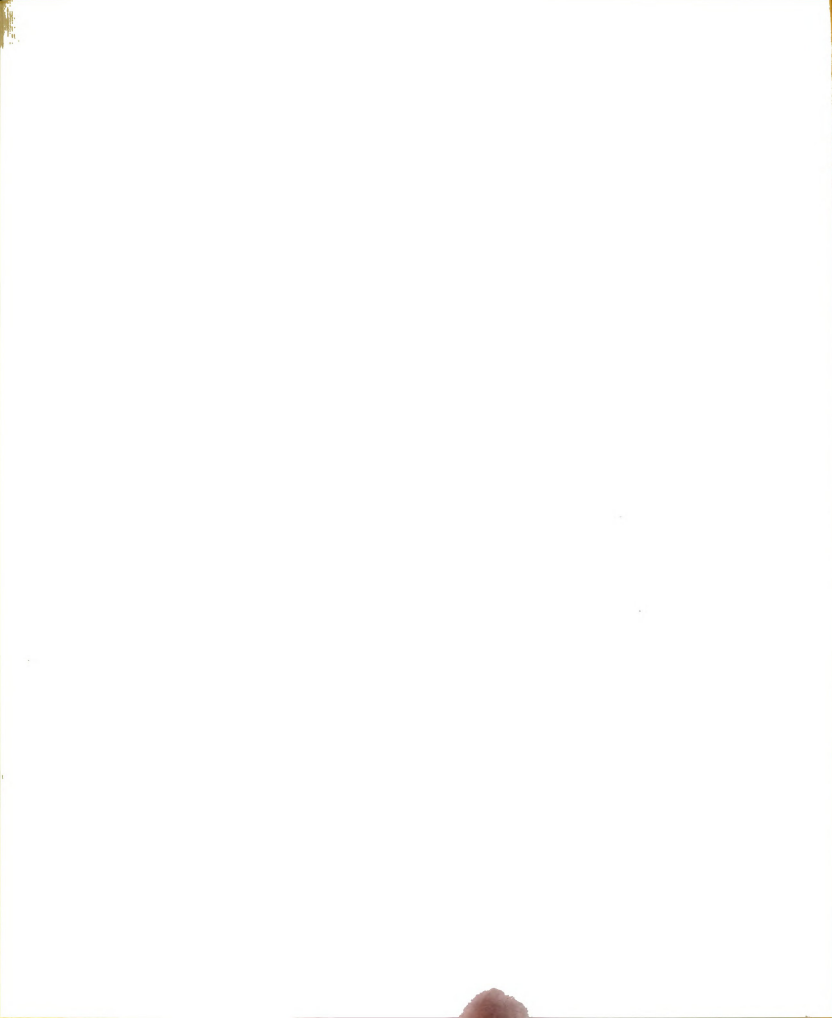
[3/2, 1/2, M]	=1.000[1/2, M, 3/2>	+0.000[1/2, M, 1/2>
[3/2, 3/2, M]	=1.000[3/2, M, 3/2>	+0.024[3/2, M, 1/2>
[3/2, 5/2, M]	=0.999[5/2, M, 3/2>	+0.040[5/2, M, 1/2>
[3/2, 7/2, M]	=0.999[7/2, M, 3/2>	+0.054[7/2, M, 1/2>
[3/2, 9/2, M]	=0.998[9/2, M, 3/2>	+0.068[9/2, M, 1/2>
[3/2, 11/2, M]	=0.997[11/2, M, 3/2>	+0.082[11/2, M, 1/2>
[3/2, 13/2, M]	=0.995[13/2, M, 3/2>	+0.096[13/2, M, 1/2>
[3/2, 15/2, M]	=0.994[15/2, M, 3/2>	+0.109[15/2, M, 1/2>
[3/2, 17/2, M]	=0.992[17/2, M, 3/2>	+0.123[17/2, M, 1/2>
[3/2, 19/2, M]	=0.991[19/2, M, 3/2>	+0.136[19/2, M, 1/2>
[3/2, 21/2, M]	=0.989[21/2, M, 3/2>	+0.149[21/2, M, 1/2>
[3/2, 23/2, M]	=0.987[23/2, M, 3/2>	+0.161[23/2, M, 1/2>
[3/2, 25/2, M]	=0.985[25/2, M, 3/2>	+0.174[25/2, M, 1/2>
[3/2, 27/2, M]	=0.983[27/2, M, 3/2>	+0.186[27/2, M, 1/2>
[3/2, 29/2, M]	=0.980[29/2, M, 3/2>	+0.198[29/2, M, 1/2>
[3/2, 31/2, M]	=0.978[31/2, M, 3/2>	+0.209[31/2, M, 1/2>
[3/2, 33/2, M]	=0.975[33/2, M, 3/2>	+0.221[33/2, M, 1/2>
[3/2, 35/2, M]	=0.973[35/2, M, 3/2>	+0.232[35/2, M, 1/2>
[3/2, 37/2, M]	=0.970[37/2, M, 3/2>	+0.242[37/2, M, 1/2>
[3/2, 39/2, M]	=0.968[39/2, M, 3/2>	+0.253[39/2, M, 1/2>
[3/2, 41/2, M]	=0.965[41/2, M, 3/2>	+0.263[41/2, M, 1/2>
[3/2, 43/2, M]	=0.962[43/2, M, 3/2>	+0.273[43/2, M, 1/2>
[3/2, 45/2, M]	=0.959[45/2, M, 3/2>	+0.283[45/2, M, 1/2>
[3/2, 47/2, M]	=0.956[47/2, M, 3/2>	+0.292[47/2, M, 1/2>
[3/2, 49/2, M]	=0.954[49/2, M, 3/2>	+0.301[49/2, M, 1/2>



APPENDIX II-B

INTERMEDIATE WAVE FUNCTIONS FOR THE
2 PI 1/2, v=0 STATE OF 15N16O AS A FUNCTION OF J

[S,J,M)		A	[J,M,S>	-	B	[J,M,S>
[1/2, 1/2,M)		=1.000	[1/2,M,1/2>	-0.000	[1/2,M,3/2>	
[1/2, 3/2,M)		=1.000	[3/2,M,1/2>	-0.024	[3/2,M,3/2>	
[1/2, 5/2,M)		=0.999	[5/2,M,1/2>	-0.039	[5/2,M,3/2>	
[1/2, 7/2,M)		=0.999	[7/2,M,1/2>	-0.053	[7/2,M,3/2>	
[1/2, 9/2,M)		=0.998	[9/2,M,1/2>	-0.066	[9/2,M,3/2>	
[1/2,11/2,M)		=0.997	[11/2,M,1/2>	-0.080	[11/2,M,3/2>	
[1/2,13/2,M)		=0.996	[13/2,M,1/2>	-0.093	[13/2,M,3/2>	
[1/2,15/2,M)		=0.994	[15/2,M,1/2>	-0.106	[15/2,M,3/2>	
[1/2,17/2,M)		=0.993	[17/2,M,1/2>	-0.119	[17/2,M,3/2>	
[1/2,19/2,M)		=0.991	[19/2,M,1/2>	-0.132	[19/2,M,3/2>	
[1/2,21/2,M)		=0.989	[21/2,M,1/2>	-0.145	[21/2,M,3/2>	
[1/2,23/2,M)		=0.988	[23/2,M,1/2>	-0.157	[23/2,M,3/2>	
[1/2,25/2,M)		=0.986	[25/2,M,1/2>	-0.169	[25/2,M,3/2>	
[1/2,27/2,M)		=0.983	[27/2,M,1/2>	-0.181	[27/2,M,3/2>	
[1/2,29/2,M)		=0.981	[29/2,M,1/2>	-0.193	[29/2,M,3/2>	
[1/2,31/2,M)		=0.979	[31/2,M,1/2>	-0.204	[31/2,M,3/2>	
[1/2,33/2,M)		=0.977	[33/2,M,1/2>	-0.215	[33/2,M,3/2>	
[1/2,35/2,M)		=0.974	[35/2,M,1/2>	-0.226	[35/2,M,3/2>	
[1/2,37/2,M)		=0.972	[37/2,M,1/2>	-0.237	[37/2,M,3/2>	
[1/2,39/2,M)		=0.969	[39/2,M,1/2>	-0.247	[39/2,M,3/2>	
[1/2,41/2,M)		=0.966	[41/2,M,1/2>	-0.257	[41/2,M,3/2>	
[1/2,43/2,M)		=0.964	[43/2,M,1/2>	-0.267	[43/2,M,3/2>	
[1/2,45/2,M)		=0.961	[45/2,M,1/2>	-0.276	[45/2,M,3/2>	
[1/2,47/2,M)		=0.958	[47/2,M,1/2>	-0.286	[47/2,M,3/2>	
[1/2,49/2,M)		=0.956	[49/2,M,1/2>	-0.295	[49/2,M,3/2>	
[1/2,51/2,M)		=0.953	[51/2,M,1/2>	-0.303	[51/2,M,3/2>	



INTERMEDIATE WAVE FUNCTIONS FOR THE
2 PI 3/2, V=0 STATE OF 15N16O AS A FUNCTION OF J

$[S, J, M)$	=	A	$[J, M, S>$	+	B	$[J, M, S>$
$[3/2, 1/2, M)$	=	1.000	$[1/2, M, 3/2>$	+	0.000	$[1/2, M, 1/2>$
$[3/2, 3/2, M)$	=	1.000	$[3/2, M, 3/2>$	+	0.024	$[3/2, M, 1/2>$
$[3/2, 5/2, M)$	=	0.999	$[5/2, M, 3/2>$	+	0.039	$[5/2, M, 1/2>$
$[3/2, 7/2, M)$	=	0.999	$[7/2, M, 3/2>$	+	0.053	$[7/2, M, 1/2>$
$[3/2, 9/2, M)$	=	0.998	$[9/2, M, 3/2>$	+	0.066	$[9/2, M, 1/2>$
$[3/2, 11/2, M)$	=	0.997	$[11/2, M, 3/2>$	+	0.080	$[11/2, M, 1/2>$
$[3/2, 13/2, M)$	=	0.996	$[13/2, M, 3/2>$	+	0.093	$[13/2, M, 1/2>$
$[3/2, 15/2, M)$	=	0.994	$[15/2, M, 3/2>$	+	0.106	$[15/2, M, 1/2>$
$[3/2, 17/2, M)$	=	0.993	$[17/2, M, 3/2>$	+	0.119	$[17/2, M, 1/2>$
$[3/2, 19/2, M)$	=	0.991	$[19/2, M, 3/2>$	+	0.132	$[19/2, M, 1/2>$
$[3/2, 21/2, M)$	=	0.989	$[21/2, M, 3/2>$	+	0.145	$[21/2, M, 1/2>$
$[3/2, 23/2, M)$	=	0.988	$[23/2, M, 3/2>$	+	0.157	$[23/2, M, 1/2>$
$[3/2, 25/2, M)$	=	0.986	$[25/2, M, 3/2>$	+	0.169	$[25/2, M, 1/2>$
$[3/2, 27/2, M)$	=	0.983	$[27/2, M, 3/2>$	+	0.181	$[27/2, M, 1/2>$
$[3/2, 29/2, M)$	=	0.981	$[29/2, M, 3/2>$	+	0.193	$[29/2, M, 1/2>$
$[3/2, 31/2, M)$	=	0.979	$[31/2, M, 3/2>$	+	0.204	$[31/2, M, 1/2>$
$[3/2, 33/2, M)$	=	0.977	$[33/2, M, 3/2>$	+	0.215	$[33/2, M, 1/2>$
$[3/2, 35/2, M)$	=	0.974	$[35/2, M, 3/2>$	+	0.226	$[35/2, M, 1/2>$
$[3/2, 37/2, M)$	=	0.972	$[37/2, M, 3/2>$	+	0.237	$[37/2, M, 1/2>$
$[3/2, 39/2, M)$	=	0.969	$[39/2, M, 3/2>$	+	0.247	$[39/2, M, 1/2>$
$[3/2, 41/2, M)$	=	0.966	$[41/2, M, 3/2>$	+	0.257	$[41/2, M, 1/2>$
$[3/2, 43/2, M)$	=	0.964	$[43/2, M, 3/2>$	+	0.267	$[43/2, M, 1/2>$
$[3/2, 45/2, M)$	=	0.961	$[45/2, M, 3/2>$	+	0.276	$[45/2, M, 1/2>$
$[3/2, 47/2, M)$	=	0.958	$[47/2, M, 3/2>$	+	0.286	$[47/2, M, 1/2>$
$[3/2, 49/2, M)$	=	0.956	$[49/2, M, 3/2>$	+	0.295	$[49/2, M, 1/2>$
$[3/2, 51/2, M)$	=	0.953	$[51/2, M, 3/2>$	+	0.303	$[51/2, M, 1/2>$

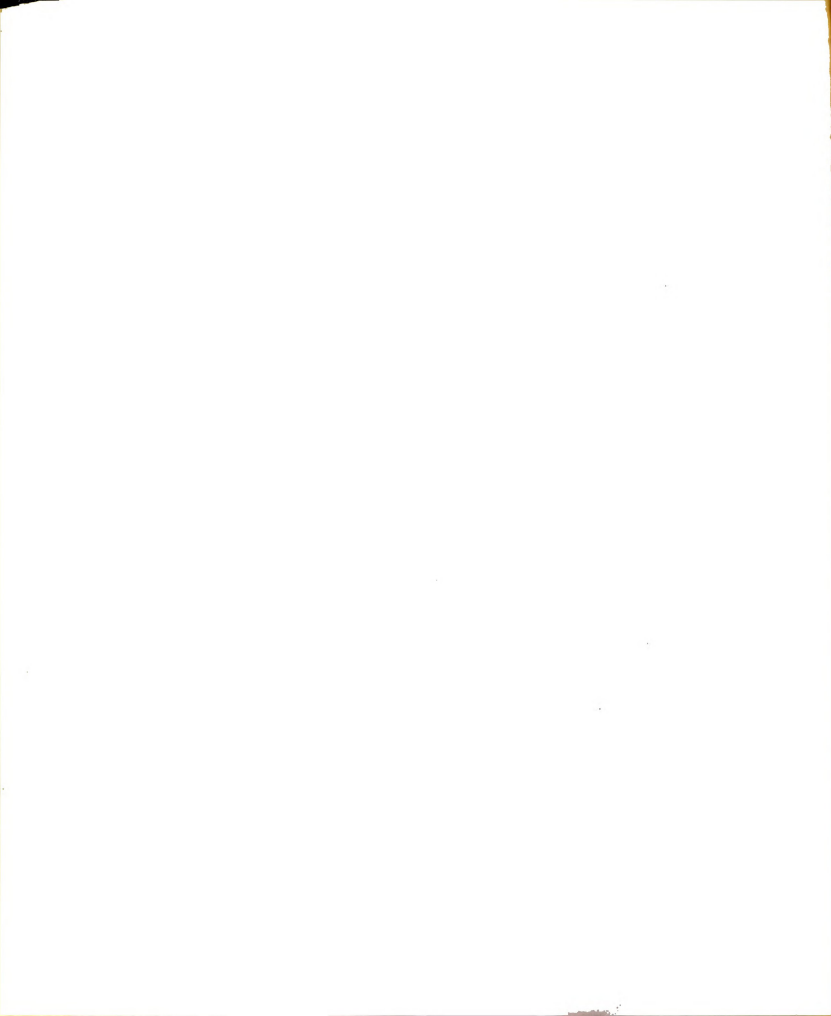


INTERMEDIATE WAVE FUNCTIONS FOR THE
2 PI 1/2, v=1 STATE OF 15N16O AS A FUNCTION OF J

[S,J,M)	=	A	(J,M,S)	=	B	(J,M,S)
[1/2, 1/2,M)	=	1.000	[1/2,M,1/2>	=	-0.000	[1/2,M,3/2>
[1/2, 3/2,M)	=	1.000	[3/2,M,1/2>	=	-0.023	[3/2,M,3/2>
[1/2, 5/2,M)	=	0.999	[5/2,M,1/2>	=	-0.038	[5/2,M,3/2>
[1/2, 7/2,M)	=	0.999	[7/2,M,1/2>	=	-0.052	[7/2,M,3/2>
[1/2, 9/2,M)	=	0.998	[9/2,M,1/2>	=	-0.066	[9/2,M,3/2>
[1/2,11/2,M)	=	0.997	[11/2,M,1/2>	=	-0.079	[11/2,M,3/2>
[1/2,13/2,M)	=	0.996	[13/2,M,1/2>	=	-0.093	[13/2,M,3/2>
[1/2,15/2,M)	=	0.994	[15/2,M,1/2>	=	-0.106	[15/2,M,3/2>
[1/2,17/2,M)	=	0.993	[17/2,M,1/2>	=	-0.118	[17/2,M,3/2>
[1/2,19/2,M)	=	0.991	[19/2,M,1/2>	=	-0.131	[19/2,M,3/2>
[1/2,21/2,M)	=	0.990	[21/2,M,1/2>	=	-0.144	[21/2,M,3/2>
[1/2,23/2,M)	=	0.988	[23/2,M,1/2>	=	-0.156	[23/2,M,3/2>
[1/2,25/2,M)	=	0.986	[25/2,M,1/2>	=	-0.168	[25/2,M,3/2>
[1/2,27/2,M)	=	0.984	[27/2,M,1/2>	=	-0.180	[27/2,M,3/2>
[1/2,29/2,M)	=	0.982	[29/2,M,1/2>	=	-0.191	[29/2,M,3/2>
[1/2,31/2,M)	=	0.979	[31/2,M,1/2>	=	-0.203	[31/2,M,3/2>
[1/2,33/2,M)	=	0.977	[33/2,M,1/2>	=	-0.214	[33/2,M,3/2>
[1/2,35/2,M)	=	0.974	[35/2,M,1/2>	=	-0.224	[35/2,M,3/2>
[1/2,37/2,M)	=	0.972	[37/2,M,1/2>	=	-0.235	[37/2,M,3/2>
[1/2,39/2,M)	=	0.969	[39/2,M,1/2>	=	-0.245	[39/2,M,3/2>
[1/2,41/2,M)	=	0.967	[41/2,M,1/2>	=	-0.255	[41/2,M,3/2>
[1/2,43/2,M)	=	0.964	[43/2,M,1/2>	=	-0.265	[43/2,M,3/2>
[1/2,45/2,M)	=	0.962	[45/2,M,1/2>	=	-0.275	[45/2,M,3/2>
[1/2,47/2,M)	=	0.959	[47/2,M,1/2>	=	-0.284	[47/2,M,3/2>
[1/2,49/2,M)	=	0.956	[49/2,M,1/2>	=	-0.293	[49/2,M,3/2>
[1/2,51/2,M)	=	0.953	[51/2,M,1/2>	=	-0.302	[51/2,M,3/2>

INTERMEDIATE WAVE FUNCTIONS FOR THE
2 PI 3/2, V=1 STATE OF 15N16O AS A FUNCTION OF J

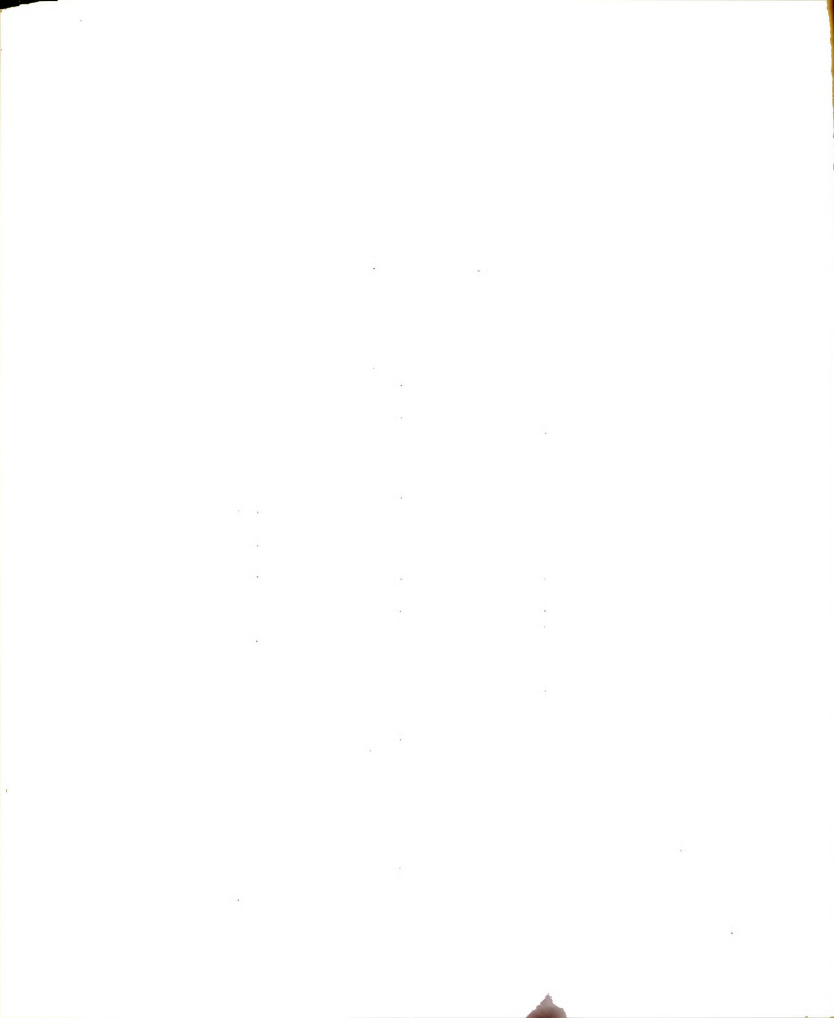
(S,J,M)	=	A	(J,M,S)	+	B	(J,M,S)
(3/2, 1/2,M)	=	1.000	(1/2,M,3/2)	+	0.000	(1/2,M,1/2)
(3/2, 3/2,M)	=	1.000	(3/2,M,3/2)	+	0.023	(3/2,M,1/2)
(3/2, 5/2,M)	=	0.999	(5/2,M,3/2)	+	0.038	(5/2,M,1/2)
(3/2, 7/2,M)	=	0.999	(7/2,M,3/2)	+	0.052	(7/2,M,1/2)
(3/2, 9/2,M)	=	0.998	(9/2,M,3/2)	+	0.066	(9/2,M,1/2)
(3/2,11/2,M)	=	0.997	(11/2,M,3/2)	+	0.079	(11/2,M,1/2)
(3/2,13/2,M)	=	0.996	(13/2,M,3/2)	+	0.093	(13/2,M,1/2)
(3/2,15/2,M)	=	0.994	(15/2,M,3/2)	+	0.106	(15/2,M,1/2)
(3/2,17/2,M)	=	0.993	(17/2,M,3/2)	+	0.118	(17/2,M,1/2)
(3/2,19/2,M)	=	0.991	(19/2,M,3/2)	+	0.131	(19/2,M,1/2)
(3/2,21/2,M)	=	0.990	(21/2,M,3/2)	+	0.144	(21/2,M,1/2)
(3/2,23/2,M)	=	0.988	(23/2,M,3/2)	+	0.156	(23/2,M,1/2)
(3/2,25/2,M)	=	0.986	(25/2,M,3/2)	+	0.168	(25/2,M,1/2)
(3/2,27/2,M)	=	0.984	(27/2,M,3/2)	+	0.180	(27/2,M,1/2)
(3/2,29/2,M)	=	0.982	(29/2,M,3/2)	+	0.191	(29/2,M,1/2)
(3/2,31/2,M)	=	0.979	(31/2,M,3/2)	+	0.203	(31/2,M,1/2)
(3/2,33/2,M)	=	0.977	(33/2,M,3/2)	+	0.214	(33/2,M,1/2)
(3/2,35/2,M)	=	0.974	(35/2,M,3/2)	+	0.224	(35/2,M,1/2)
(3/2,37/2,M)	=	0.972	(37/2,M,3/2)	+	0.235	(37/2,M,1/2)
(3/2,39/2,M)	=	0.969	(39/2,M,3/2)	+	0.245	(39/2,M,1/2)
(3/2,41/2,M)	=	0.967	(41/2,M,3/2)	+	0.255	(41/2,M,1/2)
(3/2,43/2,M)	=	0.964	(43/2,M,3/2)	+	0.265	(43/2,M,1/2)
(3/2,45/2,M)	=	0.962	(45/2,M,3/2)	+	0.275	(45/2,M,1/2)
(3/2,47/2,M)	=	0.959	(47/2,M,3/2)	+	0.284	(47/2,M,1/2)
(3/2,49/2,M)	=	0.956	(49/2,M,3/2)	+	0.293	(49/2,M,1/2)
(3/2,51/2,M)	=	0.953	(51/2,M,3/2)	+	0.302	(51/2,M,1/2)



APPENDIX III-A

CALCULATED LINE-STRENGTHS FOR 14N16O

J	P1	BRANCH Q1	R1
1/2	0,0000	0,6666	1,3325
3/2	1,3325	0,2673	2,3985
5/2	2,3985	0,1725	3,4264
7/2	3,4264	0,1285	4,4416
9/2	4,4417	0,1029	5,4511
11/2	5,4512	0,0862	6,4575
13/2	6,4576	0,0745	7,4621
15/2	7,4621	0,0658	8,4654
17/2	8,4655	0,0592	9,4680
19/2	9,4681	0,0540	10,4700
21/2	10,4701	0,0497	11,4716
23/2	11,4717	0,0463	12,4728
25/2	12,4730	0,0434	13,4739
27/2	13,4741	0,0410	14,4748
29/2	14,4750	0,0389	15,4755
31/2	15,4758	0,0371	16,4761
33/2	16,4764	0,0355	17,4767
35/2	17,4770	0,0342	18,4771
37/2	18,4775	0,0330	19,4775
39/2	19,4779	0,0319	20,4779
41/2	20,4783	0,0310	21,4783
43/2	21,4787	0,0301	22,4786
45/2	22,4790	0,0294	23,4788
47/2	23,4793	0,0287	24,4791
49/2	24,4795	0,0280	25,4793
51/2	25,4798	0,0275	26,4796
	P2	Q2	R2
3/2	0,0000	2,3980	1,6003
5/2	1,6003	1,5395	2,8576
7/2	2,8576	1,1383	4,0006
9/2	4,0007	0,9033	5,0917
11/2	5,0918	0,7483	6,1548
13/2	6,1549	0,6381	7,2012



15/2	7,2012	0,5555	8,2366
17/2	8,2367	0,4913	9,2647
19/2	9,2648	0,4399	10,2874
21/2	10,2875	0,3977	11,3062
23/2	11,3064	0,3625	12,3220
25/2	12,3222	0,3326	13,3355
27/2	13,3357	0,3069	14,3472
29/2	14,3474	0,2846	15,3573
31/2	15,3576	0,2651	16,3663
33/2	16,3666	0,2477	17,3743
35/2	17,3746	0,2323	18,3814
37/2	18,3817	0,2185	19,3878
39/2	19,3881	0,2061	20,3936
41/2	20,3939	0,1948	21,3988
43/2	21,3992	0,1845	22,4036
45/2	22,4040	0,1751	23,4080
47/2	23,4084	0,1666	24,4120
49/2	24,4125	0,1587	25,4158
51/2	25,4162	0,1514	26,4192

PH

QH

RH

1/2	0.000+000	0,000+000	8,041-004
3/2	0.000+000	6,390=004	9,634-004
5/2	2.402-003	1,091=003	1,141-003
7/2	7,776-003	1,507=003	1,321-003
9/2	1.680-002	1,904=003	1,497-003
11/2	3,003-002	2,288=003	1,665-003
13/2	4,784-002	2,657=003	1,825-003
15/2	7.048-002	3,013=003	1,973-003
17/2	9.805-002	3,354=003	2,110-003
19/2	1.305-001	3,681=003	2,234-003
21/2	1.677-001	3,992=003	2,345-003
23/2	2.095-001	4,287=003	2,443-003
25/2	2,555-001	4,566=003	2,527-003
27/2	3.053-001	4,828=003	2,598-003
29/2	3,585-001	5,074=003	2,657-003
31/2	4,146-001	5,302=003	2,703-003
33/2	4,733-001	5,514=003	2,737-003
35/2	5,340-001	5,710=003	2,760-003
37/2	5,963-001	5,890=003	2,772-003
39/2	6,596-001	6,054=003	2,776-003
41/2	7,237-001	6,204=003	2,770-003
43/2	7,880-001	6,338=003	2,756-003
45/2	8,522-001	6,459=003	2,735-003
47/2	9,159-001	6,567=003	2,708-003
49/2	9,789-001	6,662=003	2,675-003
51/2	1.041+000	6,745=003	2,638-003

PL

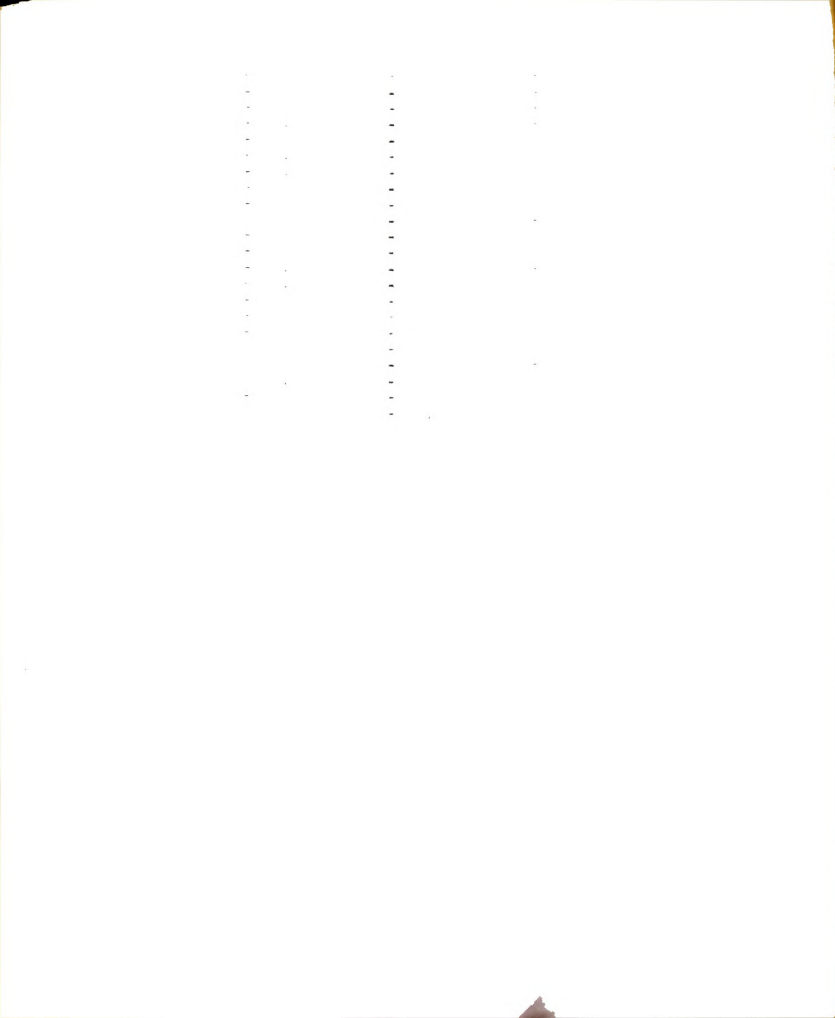
QL

RL

3/2	8.009-004	6,442=004	1,612-004
5/2	9,518-004	1,100=003	3,433-004
7/2	1,119-003	1,519=003	5,290-004

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272	273	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370	371	372	373	374	375	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442	443	444	445	446	447	448	449	450	451	452	453	454	455	456	457	458	459	460	461	462	463	464	465	466	467	468	469	470	471	472	473	474	475	476	477	478	479	480	481	482	483	484	485	486	487	488	489	490	491	492	493	494	495	496	497	498	499	500	501	502	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521	522	523	524	525	526	527	528	529	530	531	532	533	534	535	536	537	538	539	540	541	542	543	544	545	546	547	548	549	550	551	552	553	554	555	556	557	558	559	560	561	562	563	564	565	566	567	568	569	570	571	572	573	574	575	576	577	578	579	580	581	582	583	584	585	586	587	588	589	590	591	592	593	594	595	596	597	598	599	600	601	602	603	604	605	606	607	608	609	610	611	612	613	614	615	616	617	618	619	620	621	622	623	624	625	626	627	628	629	630	631	632	633	634	635	636	637	638	639	640	641	642	643	644	645	646	647	648	649	650	651	652	653	654	655	656	657	658	659	660	661	662	663	664	665	666	667	668	669	670	671	672	673	674	675	676	677	678	679	680	681	682	683	684	685	686	687	688	689	690	691	692	693	694	695	696	697	698	699	700	701	702	703	704	705	706	707	708	709	710	711	712	713	714	715	716	717	718	719	720	721	722	723	724	725	726	727	728	729	730	731	732	733	734	735	736	737	738	739	740	741	742	743	744	745	746	747	748	749	750	751	752	753	754	755	756	757	758	759	760	761	762	763	764	765	766	767	768	769	770	771	772	773	774	775	776	777	778	779	780	781	782	783	784	785	786	787	788	789	790	791	792	793	794	795	796	797	798	799	800	801	802	803	804	805	806	807	808	809	810	811	812	813	814	815	816	817	818	819	820	821	822	823	824	825	826	827	828	829	830	831	832	833	834	835	836	837	838	839	840	841	842	843	844	845	846	847	848	849	850	851	852	853	854	855	856	857	858	859	860	861	862	863	864	865	866	867	868	869	870	871	872	873	874	875	876	877	878	879	880	881	882	883	884	885	886	887	888	889	890	891	892	893	894	895	896	897	898	899	900	901	902	903	904	905	906	907	908	909	910	911	912	913	914	915	916	917	918	919	920	921	922	923	924	925	926	927	928	929	930	931	932	933	934	935	936	937	938	939	940	941	942	943	944	945	946	947	948	949	950	951	952	953	954	955	956	957	958	959	960	961	962	963	964	965	966	967	968	969	970	971	972	973	974	975	976	977	978	979	980	981	982	983	984	985	986	987	988	989	990	991	992	993	994	995	996	997	998	999	1000	1001	1002	1003	1004	1005	1006	1007	1008	1009	1010	1011	1012	1013	1014	1015	1016	1017	1018	1019	1020	1021	1022	1023	1024	1025	1026	1027	1028	1029	1030	1031	1032	1033	1034	1035	1036	1037	1038	1039	1040	1041	1042	1043	1044	1045	1046	1047	1048	1049	1050	1051	1052	1053	1054	1055	1056	1057	1058	1059	1060	1061	1062	1063	1064	1065	1066	1067	1068	1069	1070	1071	1072	1073	1074	1075	1076	1077	1078	1079	1080	1081	1082	1083	1084	1085	1086	1087	1088	1089	1090	1091	1092	1093	1094	1095	1096	1097	1098	1099	1100	1101	1102	1103	1104	1105	1106	1107	1108	1109	1110	1111	1112	1113	1114	1115	1116	1117	1118	1119	1120	1121	1122	1123	1124	1125	1126	1127	1128	1129	1130	1131	1132	1133	1134	1135	1136	1137	1138	1139	1140	1141	1142	1143	1144	1145	1146	1147	1148	1149	1150	1151	1152	1153	1154	1155	1156	1157	1158	1159	1160	1161	1162	1163	1164	1165	1166	1167	1168	1169	1170	1171	1172	1173	1174	1175	1176	1177	1178	1179	1180	1181	1182	1183	1184	1185	1186	1187	1188	1189	1190	1191	1192	1193	1194	1195	1196	1197	1198	1199	1200	1201	1202	1203	1204	1205	1206	1207	1208	1209	1210	1211	1212	1213	1214	1215	1216	1217	1218	1219	1220	1221	1222	1223	1224	1225	1226	1227	1228	1229	1230	1231	1232	1233	1234	1235	1236	1237	1238	1239	1240	1241	1242	1243	1244	1245	1246	1247	1248	1249	1250	1251	1252	1253	1254	1255	1256	1257	1258	1259	1260	1261	1262	1263	1264	1265	1266	1267	1268	1269	1270	1271	1272	1273	1274	1275	1276	1277	1278	1279	1280	1281	1282	1283	1284	1285	1286	1287	1288	1289	1290	1291	1292	1293	1294	1295	1296	1297	1298	1299	1300	1301	1302	1303	1304	1305	1306	1307	1308	1309	1310	1311	1312	1313	1314	1315	1316	1317	1318	1319	1320	1321	1322	1323	1324	1325	1326	1327	1328	1329	1330	1331	1332	1333	1334	1335	1336	1337	1338	1339	1340	1341	1342	1343	1344	1345	1346	1347	1348	1349	1350	1351	1352	1353	1354	1355	1356	1357	1358	1359	1360	1361	1362	1363	1364	1365	1366	1367	1368	1369	1370	1371	1372	1373	1374	1375	1376	1377	1378	1379	1380	1381	1382	1383	1384	1385	1386	1387	1388	1389	1390	1391	1392	1393	1394	1395	1396	1397	1398	1399	1400	1401	1402	1403	1404	1405	1406	1407	1408	1409	1410	1411	1412	1413	1414	1415	1416	1417	1418	1419	1420	1421	1422	1423	1424	1425	1426	1427	1428	1429	1430	1431	1432	1433	1434	1435	1436	1437	1438	1439	1440	1441	1442	1443	1444	1445	1446	1447	1448	1449	1450	1451	1452	1453	1454	1455	1456	1457	1458	1459	1460	1461	1462	1463	1464	1465	1466	1467	1468	1469	1470	1471	1472	1473	1474	1475	1476	1477	1478	1479	1480	1481	1482	1483	1484	1485	1486	1487	1488	1489	1490	1491	1492	1493	1494	1495	14
---	---	---	---	---	---	---	---	---	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	----

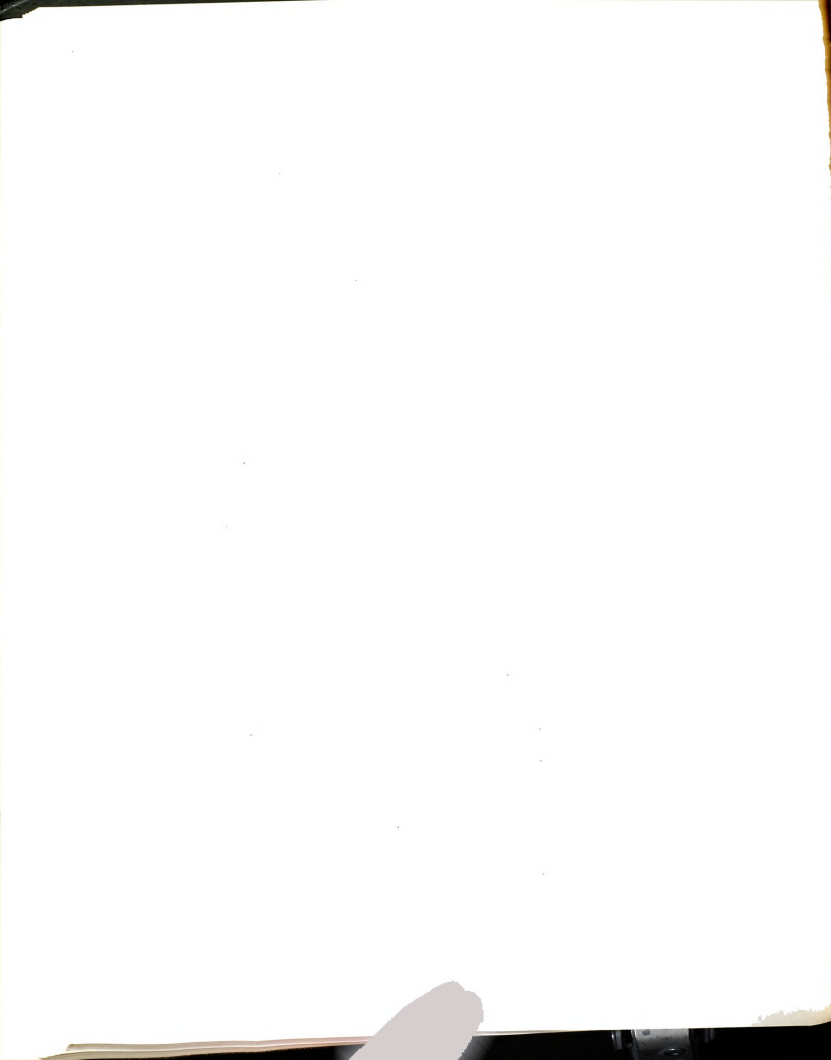
9/2	1.284-003	1,920-003	7,123-004
11/2	1.444-003	2,306-003	8,902-004
13/2	1.593-003	2,678-003	1,060-003
15/2	1.731-003	3,037-003	1,221-003
17/2	1.857-003	3,381-003	1,372-003
19/2	1.970-003	3,710-003	1,511-003
21/2	2.069-003	4,023-003	1,637-003
23/2	2.155-003	4,320-003	1,752-003
25/2	2.227-003	4,601-003	1,854-003
27/2	2.285-003	4,865-003	1,943-003
29/2	2,331-003	5,111-003	2,020-003
31/2	2,364-003	5,341-003	2,085-003
33/2	2,386-003	5,555-003	2,138-003
35/2	2,397-003	5,751-003	2,180-003
37/2	2,398-003	5,932-003	2,212-003
39/2	2,390-003	6,097-003	2,234-003
41/2	2,373-003	6,247-003	2,247-003
43/2	2,350-003	6,382-003	2,252-003
45/2	2,320-003	6,503-003	2,250-003
47/2	2,284-003	6,611-003	2,240-003
49/2	2,243-003	6,706-003	2,225-003
51/2	2,198-003	6,789-003	2,205-003



APPENDIX III-B

CALCULATED LINE-STRENGTHS FOR 15N16O

J	P1	BRANCH Q1	R1
1/2	0,0000	0,6666	1,3326
3/2	1,3325	0,2672	2,3986
5/2	2,3986	0,1724	3,4266
7/2	3,4265	0,1284	4,4419
9/2	4,4418	0,1028	5,4515
11/2	5,4513	0,0861	6,4580
13/2	6,4577	0,0745	7,4626
15/2	7,4623	0,0656	8,4660
17/2	8,4656	0,0589	9,4687
19/2	9,4682	0,0537	10,4708
21/2	10,4702	0,0494	11,4724
23/2	11,4718	0,0459	12,4738
25/2	12,4730	0,0430	13,4749
27/2	13,4740	0,0406	14,4759
29/2	14,4749	0,0385	15,4767
31/2	15,4756	0,0367	16,4774
33/2	16,4762	0,0351	17,4779
35/2	17,4767	0,0337	18,4785
37/2	18,4771	0,0325	19,4789
39/2	19,4775	0,0314	20,4793
41/2	20,4778	0,0305	21,4797
43/2	21,4781	0,0296	22,4801
45/2	22,4784	0,0288	23,4804
47/2	23,4786	0,0281	24,4807
49/2	24,4789	0,0275	25,4809
51/2	25,4791	0,0269	26,4812
	P2	Q2	R2
3/2	0,0000	2,3981	1,6002
5/2	1,6002	1,5398	2,8576
7/2	2,8575	1,1386	4,0006
9/2	4,0005	0,9038	5,0917
11/2	5,0916	0,7488	6,1549
13/2	6,1546	0,6387	7,2012



15/2	7,2009	0,5563	8,2367
17/2	8,2363	0,4921	9,2648
19/2	9,2643	0,4407	10,2876
21/2	10,2870	0,3986	11,3064
23/2	11,3057	0,3635	12,3223
25/2	12,3215	0,3337	13,3358
27/2	13,3349	0,3080	14,3475
29/2	14,3465	0,2858	15,3577
31/2	15,3566	0,2662	16,3667
33/2	16,3656	0,2489	17,3747
35/2	17,3735	0,2336	18,3819
37/2	18,3805	0,2198	19,3883
39/2	19,3868	0,2073	20,3941
41/2	20,3926	0,1961	21,3994
43/2	21,3978	0,1858	22,4042
45/2	22,4025	0,1764	23,4086
47/2	23,4069	0,1678	24,4127
49/2	24,4109	0,1599	25,4164
51/2	25,4146	0,1527	26,4199

PH

QH

RH

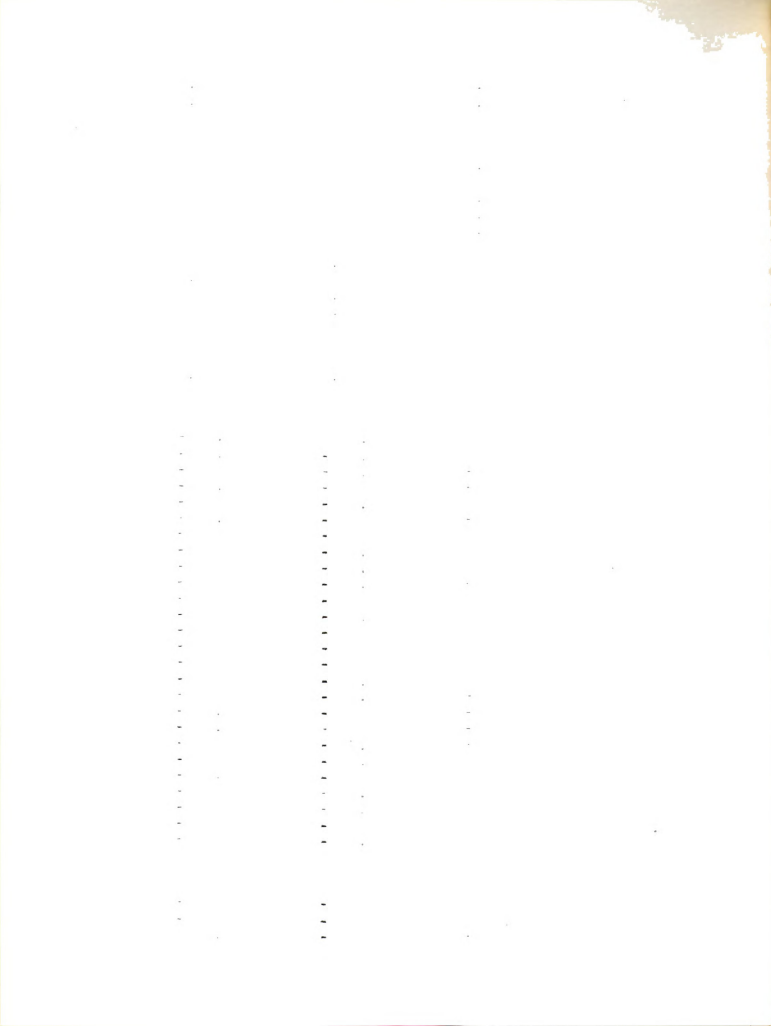
1/2	0.000+000	0,000+000	7,308-004
3/2	0.000+000	5,992=004	8,578-004
5/2	2.236-003	1,023-003	9,958-004
7/2	7.251-003	1,414-003	1,129-003
9/2	1.570-002	1,788=003	1,224-003
11/2	2.811-002	2,149=003	1,368-003
13/2	4.489-002	2,498=003	1,469-003
15/2	6.629-002	2,835=003	1,557-003
17/2	9.244-002	3,159=003	1,632-003
19/2	1.234-001	3,470=003	1,694-003
21/2	1.590-001	3,767=003	1,743-003
23/2	1.990-001	4,050=003	1,780-003
25/2	2.434-001	4,318=003	1,806-003
27/2	2.916-001	4,571=003	1,820-003
29/2	3.434-001	4,809=003	1,824-003
31/2	3.984-001	5,032=003	1,819-003
33/2	4.561-001	5,240=003	1,805-003
35/2	5.160-001	5,434=003	1,783-003
37/2	5.778-001	5,612=003	1,755-003
39/2	6.410-001	5,776=003	1,722-003
41/2	7.053-001	5,927=003	1,683-003
43/2	7.701-001	6,063=003	1,640-003
45/2	8.351-001	6,187=003	1,593-003
47/2	9.001-001	6,299=003	1,544-003
49/2	9.646-001	6,398=003	1,493-003
51/2	1.028+000	6,486=003	1,440-003

PL

QL

RL

3/2	7.432-004	5,794=004	1,376-004
5/2	9.022-004	9,896=004	2,870-004
7/2	1.083-003	1,368=003	4,332-004



9/2	1.271-003	1,729-003	5,716-004
11/2	1.459-003	2,079-003	6,998-004
13/2	1.645-003	2,416-003	8,168-004
15/2	1.827-003	2,743-003	9,218-004
17/2	2.003-003	3,057-003	1,014-003
19/2	2.172-003	3,359-003	1,095-003
21/2	2.332-003	3,647-003	1,163-003
23/2	2.482-003	3,922-003	1,219-003
25/2	2.621-003	4,183-003	1,263-003
27/2	2.750-003	4,429-003	1,297-003
29/2	2.867-003	4,662-003	1,321-003
31/2	2.972-003	4,879-003	1,335-003
33/2	3.066-003	5,083-003	1,341-003
35/2	3.147-003	5,272-003	1,358-003
37/2	3.218-003	5,447-003	1,329-003
39/2	3.277-003	5,608-003	1,314-003
41/2	3.325-003	5,756-003	1,293-003
43/2	3.363-003	5,891-003	1,268-003
45/2	3.392-003	6,013-003	1,238-003
47/2	3.411-003	6,123-003	1,206-003
49/2	3.422-003	6,222-003	1,170-003
51/2	3.424-003	6,310-003	1,133-003

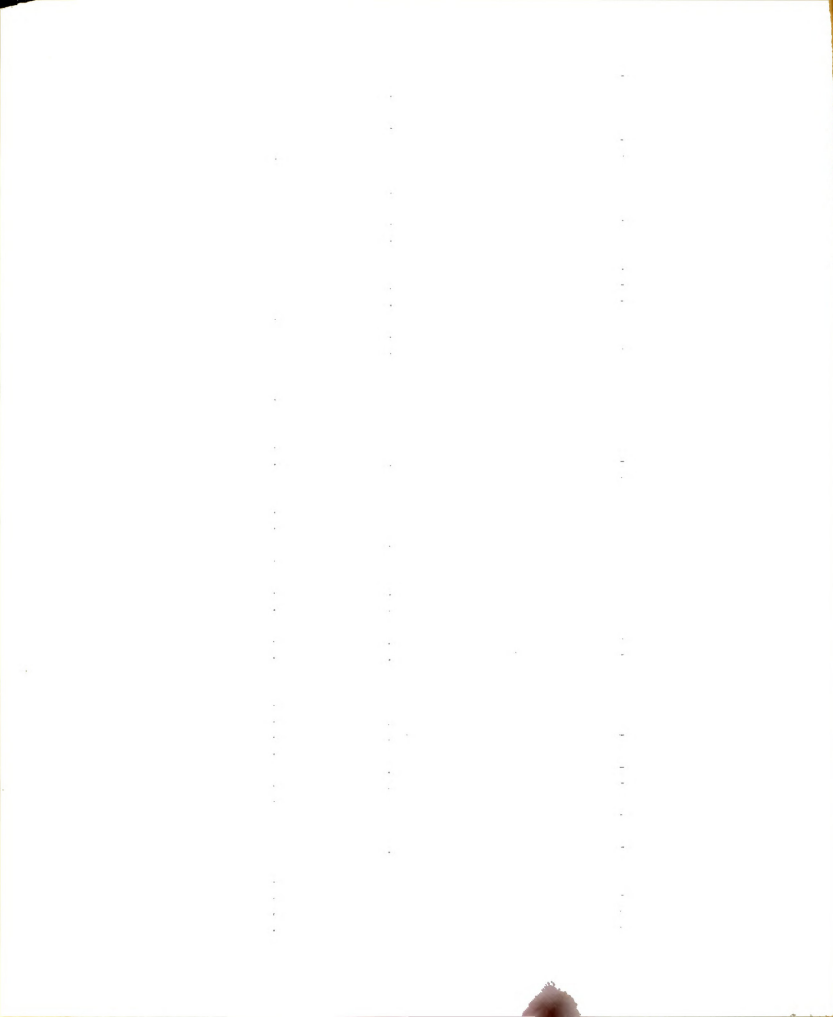
APPENDIX IV

CALCULATED VALUES FOR THE INTEGRATED ABSORPTION COEFFICIENT FOR $^{14}\text{N}^{16}\text{O}$

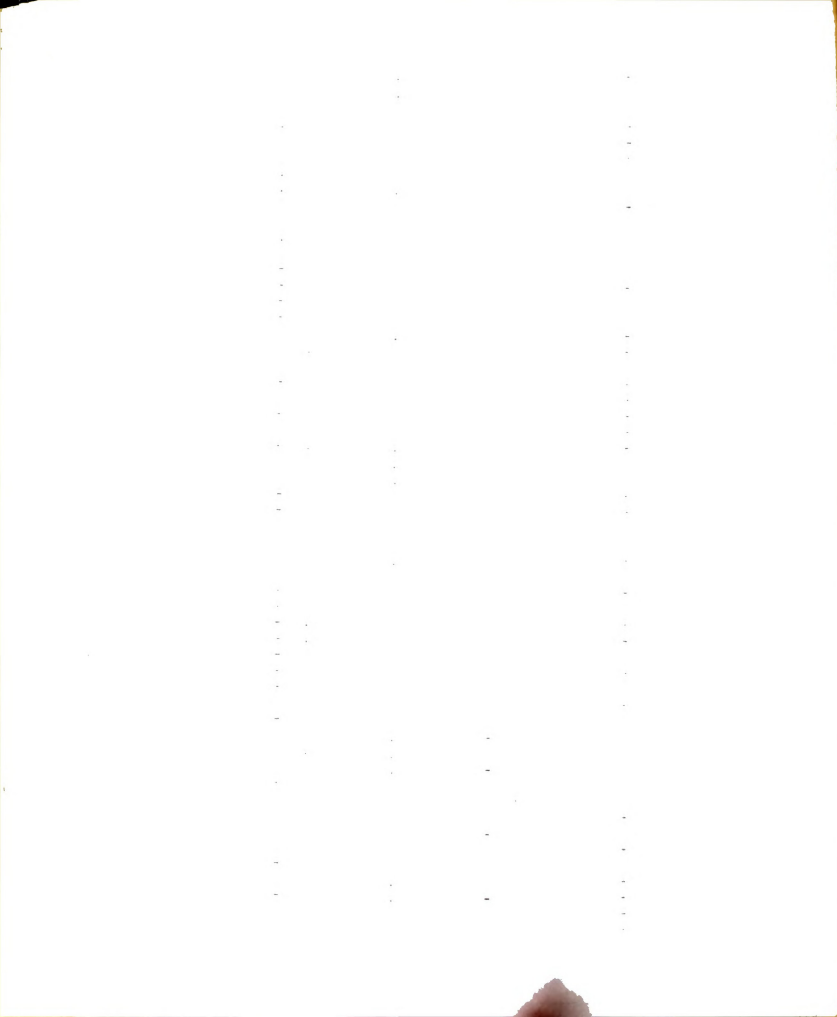
IDENTIFICATION	FREQUENCY	S ₀
1-0 N40 P1 3/2	1871,0000	0,79
1-0 N40 P1 5/2	1867,6000	1,37
1-0 N40 P1 7/2	1864,2000	1,84
1-0 N40 P1 9/2	1860,7000	2,22
1-0 N40 P1 11/2	1857,2000	2,48
1-0 N40 P1 13/2	1853,7000	2,64
1-0 N40 P1 15/2	1850,1000	2,69
1-0 N40 P1 17/2	1846,5000	2,66
1-0 N40 P1 19/2	1842,9000	2,54
1-0 N40 P1 21/2	1839,2000	2,36
1-0 N40 P1 23/2	1835,5000	2,14
1-0 N40 P1 25/2	1831,8000	1,90
1-0 N40 P1 27/2	1828,0000	1,64
1-0 N40 P1 29/2	1824,2000	1,39
1-0 N40 P1 31/2	1820,4000	1,15
1-0 N40 P1 33/2	1816,5000	0,94
1-0 N40 P1 35/2	1812,6000	0,75
1-0 N40 P1 37/2	1808,6000	0,58
1-0 N40 P1 39/2	1804,7000	0,45
1-0 N40 P1 41/2	1800,7000	0,34
1-0 N40 P1 43/2	1796,6000	0,25
1-0 N40 P1 45/2	1792,6000	0,18
1-0 N40 P1 47/2	1788,4000	0,13
1-0 N40 P1 49/2	1784,3000	0,09
1-0 N40 P1 51/2	1780,1000	0,06
1-0 N40 R1 1/2	1881,0000	0,82
1-0 N40 R1 3/2	1884,3000	1,44
1-0 N40 R1 5/2	1887,5000	1,97
1-0 N40 R1 7/2	1890,7000	2,42
1-0 N40 R1 9/2	1893,8000	2,77
1-0 N40 R1 11/2	1896,9000	3,00
1-0 N40 R1 13/2	1900,0000	3,13
1-0 N40 R1 15/2	1903,1000	3,14



1=0	N40	R1	17/2	1906,1000	3,07
1=0	N40	R1	19/2	1909,1000	2,91
1=0	N40	R1	21/2	1912,0000	2,69
1=0	N40	R1	23/2	1914,9000	2,43
1=0	N40	R1	25/2	1917,8000	2,15
1=0	N40	R1	27/2	1920,7000	1,85
1=0	N40	R1	29/2	1923,5000	1,57
1=0	N40	R1	31/2	1926,2000	1,30
1=0	N40	R1	33/2	1929,0000	1,06
1=0	N40	R1	35/2	1931,7000	0,84
1=0	N40	R1	37/2	1934,3000	0,66
1=0	N40	R1	39/2	1937,0000	0,50
1=0	N40	R1	41/2	1939,6000	0,38
1=0	N40	R1	43/2	1942,1000	0,28
1=0	N40	R1	45/2	1944,6000	0,20
1=0	N40	R1	47/2	1947,1000	0,14
1=0	N40	R1	49/2	1949,6000	0,10
1=0	N40	R1	51/2	1952,0000	0,07
1=0	N40	P2	5/2	1867,2000	0,61
1=0	N40	P2	7/2	1863,6000	1,03
1=0	N40	P2	9/2	1860,1000	1,34
1=0	N40	P2	11/2	1856,5000	1,55
1=0	N40	P2	13/2	1852,8000	1,69
1=0	N40	P2	15/2	1849,2000	1,74
1=0	N40	P2	17/2	1845,5000	1,73
1=0	N40	P2	19/2	1841,7000	1,67
1=0	N40	P2	21/2	1838,0000	1,56
1=0	N40	P2	23/2	1834,2000	1,42
1=0	N40	P2	25/2	1830,3000	1,26
1=0	N40	P2	27/2	1826,4000	1,09
1=0	N40	P2	29/2	1822,5000	0,92
1=0	N40	P2	31/2	1818,6000	0,77
1=0	N40	P2	33/2	1814,6000	0,62
1=0	N40	P2	35/2	1810,6000	0,50
1=0	N40	P2	37/2	1806,6000	0,39
1=0	N40	P2	39/2	1802,5000	0,30
1=0	N40	P2	41/2	1798,4000	0,22
1=0	N40	P2	43/2	1794,3000	0,17
1=0	N40	P2	45/2	1790,2000	0,12
1=0	N40	P2	47/2	1786,0000	0,09
1=0	N40	P2	49/2	1781,7000	0,06
1=0	N40	P2	51/2	1777,5000	0,04
1=0	N40	R2	5/2	1887,6000	1,10
1=0	N40	R2	7/2	1890,9000	1,46
1=0	N40	R2	9/2	1894,1000	1,73
1=0	N40	R2	11/2	1897,3000	1,92
1=0	N40	R2	13/2	1900,5000	2,02
1=0	N40	R2	15/2	1903,6000	2,05
1=0	N40	R2	17/2	1906,7000	2,01
1=0	N40	R2	19/2	1909,7000	1,92
1=0	N40	R2	21/2	1912,7000	1,78
1=0	N40	R2	23/2	1915,7000	1,61
1=0	N40	R2	25/2	1918,7000	1,43
1=0	N40	R2	27/2	1921,5000	1,23



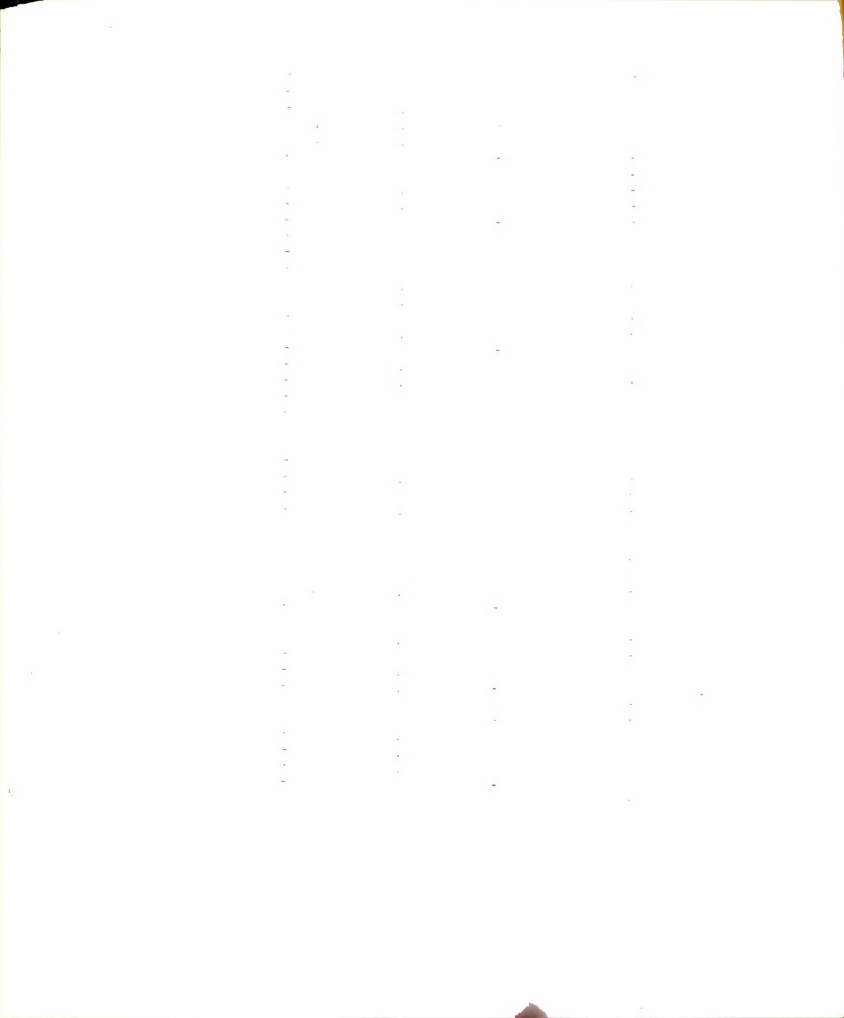
1-0 N40 R2 29/2	1924,4000	1.04
1-0 N40 R2 31/2	1927,2000	0.87
1-0 N40 R2 33/2	1930,0000	0.70
1-0 N40 R2 35/2	1932,7000	0.56
1-0 N40 R2 37/2	1935,4000	0.44
1-0 N40 R2 39/2	1938,1000	0.34
1-0 N40 R2 41/2	1940,7000	0.25
1-0 N40 R2 43/2	1943,3000	0.19
1-0 N40 R2 45/2	1945,9000	0.14
1-0 N40 R2 47/2	1948,4000	0.10
1-0 N40 R2 49/2	1950,8000	0.07
1-0 N40 R2 51/2	1953,2000	0.05
1-0 N40 PH 5/2	1987,3000	1.46-003
1-0 N40 PH 7/2	1984,1000	4.45-003
1-0 N40 PH 13/2	1974,9000	2.08-002
1-0 N40 PH 19/2-	1966,1000	1.87-002
1-0 N40 PH 19/2+	1966,2000	1.87-002
1-0 N40 PH 21/2	1963,3000	4.04-002
1-0 N40 PH 23/2-	1960,5000	2.09-002
1-0 N40 PH 23/2+	1960,7000	2.09-002
1-0 N40 PH 27/2-	1955,2000	1.99-002
1-0 N40 PH 27/2+	1955,3000	1.99-002
1-0 N40 PH 29/2-	1952,5000	1.84-002
1-0 N40 PH 29/2+	1952,7000	1.84-002
1-0 N40 PH 31/2-	1950,0000	1.66-002
1-0 N40 PH 31/2+	1950,1000	1.66-002
1-0 N40 QH 3/2	1995,7000	4.05-004
1-0 N40 QH 5/2	1995,8000	6.65-004
1-0 N40 QH 7/2	1996,0000	8.67-004
1-0 N40 QH 9/2	1996,3000	1.02-003
1-0 N40 QH 11/2	1996,6000	1.12-003
1-0 N40 QH 13/2	1997,0000	1.17-003
1-0 N40 QH 15/2-	1997,4000	5.87-004
1-0 N40 QH 15/2	1997,4000	1.17-003
1-0 N40 QH 15/2+	1997,5000	5.87-004
1-0 N40 QH 17/2-	1997,9000	5.70-004
1-0 N40 QH 17/2+	1998,0000	5.70-004
1-0 N40 QH 19/2-	1998,4000	5.36-004
1-0 N40 QH 19/2+	1998,5000	5.36-004
1-0 N40 QH 21/2-	1999,0000	4.90-004
1-0 N40 QH 21/2+	1999,1000	4.90-004
1-0 N40 QH 23/2-	1999,6000	4.36-004
1-0 N40 QH 23/2+	1999,8000	4.37-004
1-0 N40 QH 25/2-	2000,3000	3.79-004
1-0 N40 QH 25/2+	2000,4000	3.79-004
1-0 N40 QH 27/2-	2001,0000	3.22-004
1-0 N40 QH 27/2+	2001,2000	3.22-004
1-0 N40 QH 29/2-	2001,8000	2.68-004
1-0 N40 QH 29/2+	2002,0000	2.68-004
1-0 N40 QH 31/2-	2002,6000	2.17-004
1-0 N40 QH 31/2+	2002,8000	2.17-004
1-0 N40 QH 33/2-	2003,4000	1.73-004
1-0 N40 QH 33/2+	2003,6000	1.73-004
1-0 N40 QH 35/2-	2004,3000	1.35-004



1-0	N40	QH	35/2+	2004,5000	1,35-004
1-0	N40	QH	37/2-	2005,2000	1,03-004
1-0	N40	QH	37/2+	2005,4000	1,03-004
1-0	N40	QH	39/2-	2006,1000	7,71-005
1-0	N40	QH	39/2+	2006,3000	7,71-005
1-0	N40	QH	41/2-	2007,1000	5,66-005
1-0	N40	QH	41/2+	2007,3000	5,66-005
1-0	N40	QH	43/2-	2008,0000	4,08-005
1-0	N40	QH	43/2+	2008,3000	4,08-005
1-0	N40	QH	45/2-	2009,0000	2,88-005
1-0	N40	QH	45/2+	2009,3000	2,88-005
1-0	N40	QH	47/2-	2010,0000	2,00-005
1-0	N40	QH	47/2+	2010,3000	2,00-005
1-0	N40	RH	1/2	2000,7000	5,24-004
1-0	N40	RH	3/2	2004,2000	6,14-004
1-0	N40	RH	5/2	2007,7000	7,00-004
1-0	N40	RH	7/2	2011,3000	7,66-004
1-0	N40	RH	9/2	2015,0000	8,08-004
1-0	N40	RH	11/2	2018,7000	8,24-004
1-0	N40	RH	13/2	2022,5000	8,14-004
1-0	N40	RH	15/2-	2026,3000	3,90-004
1-0	N40	RH	15/2+	2026,4000	3,90-004
1-0	N40	RH	17/2-	2030,2000	3,64-004
1-0	N40	RH	17/2+	2030,3000	3,64-004
1-0	N40	RH	19/2-	2034,1000	3,31-004
1-0	N40	RH	19/2+	2034,2000	3,31-004
1-0	N40	RH	21/2-	2038,1000	2,93-004
1-0	N40	RH	21/2+	2038,2000	2,93-004
1-0	N40	RH	23/2-	2042,1000	2,54-004
1-0	N40	RH	23/2+	2042,2000	2,54-004
1-0	N40	RH	25/2-	2046,2000	2,15-004
1-0	N40	RH	25/2+	2046,3000	2,15-004
1-0	N40	RH	27/2-	2050,3000	1,78-004
1-0	N40	RH	27/2+	2050,4000	1,78-004
1-0	N40	RH	29/2-	2054,4000	1,44-004
1-0	N40	RH	29/2+	2054,6000	1,44-004
1-0	N40	RH	31/2-	2058,6000	1,14-004
1-0	N40	RH	31/2+	2058,7000	1,14-004
1-0	N40	RH	33/2-	2062,8000	8,84-005
1-0	N40	RH	33/2+	2063,0000	8,84-005
1-0	N40	RH	35/2-	2067,0000	6,72-005
1-0	N40	RH	35/2+	2067,2000	6,72-005
1-0	N40	RH	37/2-	2071,3000	5,01-005
1-0	N40	RH	37/2+	2071,5000	5,01-005
1-0	N40	RH	39/2-	2075,6000	3,66-005
1-0	N40	RH	39/2+	2075,8000	3,66-005
1-0	N40	RH	41/2-	2079,9000	2,62-005
1-0	N40	RH	41/2+	2080,1000	2,62-005
1-0	N40	PL	7/2	1743,7000	3,77-004
1-0	N40	PL	9/2	1739,8000	4,02-004
1-0	N40	PL	11/2-	1735,8000	2,06-004
1-0	N40	PL	11/2	1735,8000	4,12-004
1-0	N40	PL	13/2-	1731,6000	2,04-004
1-0	N40	PL	13/2	1731,7000	4,08-004

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272	273	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370	371	372	373	374	375	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442	443	444	445	446	447	448	449	450	451	452	453	454	455	456	457	458	459	460	461	462	463	464	465	466	467	468	469	470	471	472	473	474	475	476	477	478	479	480	481	482	483	484	485	486	487	488	489	490	491	492	493	494	495	496	497	498	499	500	501	502	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521	522	523	524	525	526	527	528	529	530	531	532	533	534	535	536	537	538	539	540	541	542	543	544	545	546	547	548	549	550	551	552	553	554	555	556	557	558	559	560	561	562	563	564	565	566	567	568	569	570	571	572	573	574	575	576	577	578	579	580	581	582	583	584	585	586	587	588	589	590	591	592	593	594	595	596	597	598	599	600	601	602	603	604	605	606	607	608	609	610	611	612	613	614	615	616	617	618	619	620	621	622	623	624	625	626	627	628	629	630	631	632	633	634	635	636	637	638	639	640	641	642	643	644	645	646	647	648	649	650	651	652	653	654	655	656	657	658	659	660	661	662	663	664	665	666	667	668	669	670	671	672	673	674	675	676	677	678	679	680	681	682	683	684	685	686	687	688	689	690	691	692	693	694	695	696	697	698	699	700	701	702	703	704	705	706	707	708	709	710	711	712	713	714	715	716	717	718	719	720	721	722	723	724	725	726	727	728	729	730	731	732	733	734	735	736	737	738	739	740	741	742	743	744	745	746	747	748	749	750	751	752	753	754	755	756	757	758	759	760	761	762	763	764	765	766	767	768	769	770	771	772	773	774	775	776	777	778	779	780	781	782	783	784	785	786	787	788	789	790	791	792	793	794	795	796	797	798	799	800	801	802	803	804	805	806	807	808	809	810	811	812	813	814	815	816	817	818	819	820	821	822	823	824	825	826	827	828	829	830	831	832	833	834	835	836	837	838	839	840	841	842	843	844	845	846	847	848	849	850	851	852	853	854	855	856	857	858	859	860	861	862	863	864	865	866	867	868	869	870	871	872	873	874	875	876	877	878	879	880	881	882	883	884	885	886	887	888	889	890	891	892	893	894	895	896	897	898	899	900	901	902	903	904	905	906	907	908	909	910	911	912	913	914	915	916	917	918	919	920	921	922	923	924	925	926	927	928	929	930	931	932	933	934	935	936	937	938	939	940	941	942	943	944	945	946	947	948	949	950	951	952	953	954	955	956	957	958	959	960	961	962	963	964	965	966	967	968	969	970	971	972	973	974	975	976	977	978	979	980	981	982	983	984	985	986	987	988	989	990	991	992	993	994	995	996	997	998	999	1000	1001	1002	1003	1004	1005	1006	1007	1008	1009	1010	1011	1012	1013	1014	1015	1016	1017	1018	1019	1020	1021	1022	1023	1024	1025	1026	1027	1028	1029	1030	1031	1032	1033	1034	1035	1036	1037	1038	1039	1040	1041	1042	1043	1044	1045	1046	1047	1048	1049	1050	1051	1052	1053	1054	1055	1056	1057	1058	1059	1060	1061	1062	1063	1064	1065	1066	1067	1068	1069	1070	1071	1072	1073	1074	1075	1076	1077	1078	1079	1080	1081	1082	1083	1084	1085	1086	1087	1088	1089	1090	1091	1092	1093	1094	1095	1096	1097	1098	1099	1100	1101	1102	1103	1104	1105	1106	1107	1108	1109	1110	1111	1112	1113	1114	1115	1116	1117	1118	1119	1120	1121	1122	1123	1124	1125	1126	1127	1128	1129	1130	1131	1132	1133	1134	1135	1136	1137	1138	1139	1140	1141	1142	1143	1144	1145	1146	1147	1148	1149	1150	1151	1152	1153	1154	1155	1156	1157	1158	1159	1160	1161	1162	1163	1164	1165	1166	1167	1168	1169	1170	1171	1172	1173	1174	1175	1176	1177	1178	1179	1180	1181	1182	1183	1184	1185	1186	1187	1188	1189	1190	1191	1192	1193	1194	1195	1196	1197	1198	1199	1200	1201	1202	1203	1204	1205	1206	1207	1208	1209	1210	1211	1212	1213	1214	1215	1216	1217	1218	1219	1220	1221	1222	1223	1224	1225	1226	1227	1228	1229	1230	1231	1232	1233	1234	1235	1236	1237	1238	1239	1240	1241	1242	1243	1244	1245	1246	1247	1248	1249	1250	1251	1252	1253	1254	1255	1256	1257	1258	1259	1260	1261	1262	1263	1264	1265	1266	1267	1268	1269	1270	1271	1272	1273	1274	1275	1276	1277	1278	1279	1280	1281	1282	1283	1284	1285	1286	1287	1288	1289	1290	1291	1292	1293	1294	1295	1296	1297	1298	1299	1300	1301	1302	1303	1304	1305	1306	1307	1308	1309	1310	1311	1312	1313	1314	1315	1316	1317	1318	1319	1320	1321	1322	1323	1324	1325	1326	1327	1328	1329	1330	1331	1332	1333	1334	1335	1336	1337	1338	1339	1340	1341	1342	1343	1344	1345	1346	1347	1348	1349	1350	1351	1352	1353	1354	1355	1356	1357	1358	1359	1360	1361	1362	1363	1364	1365	1366	1367	1368	1369	1370	1371	1372	1373	1374	1375	1376	1377	1378	1379	1380	1381	1382	1383	1384	1385	1386	1387	1388	1389	1390	1391	1392	1393	1394	1395	1396	1397	1398	1399	1400	1401	1402	1403	1404	1405	1406	1407	1408	1409	1410	1411	1412	1413	1414	1415	1416	1417	1418	1419	1420	1421	1422	1423	1424	1425	1426	1427	1428	1429	1430	1431	1432	1433	1434	1435	1436	1437	1438	1439	1440	1441	1442	1443	1444	1445	1446	1447	1448	1449	1450	1451	1452	1453	1454	1455	1456	1457	1458	1459	1460	1461	1462	1463	1464	1465	1466	1467	1468	1469	1470	1471	1472	1473	1474	1475	1476	1477	1478	1479	1480	1481	1482	1483	1484	1485	1486	1487	1488	1489	1490	1491	1492	1493	1494	1495	14
---	---	---	---	---	---	---	---	---	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	----

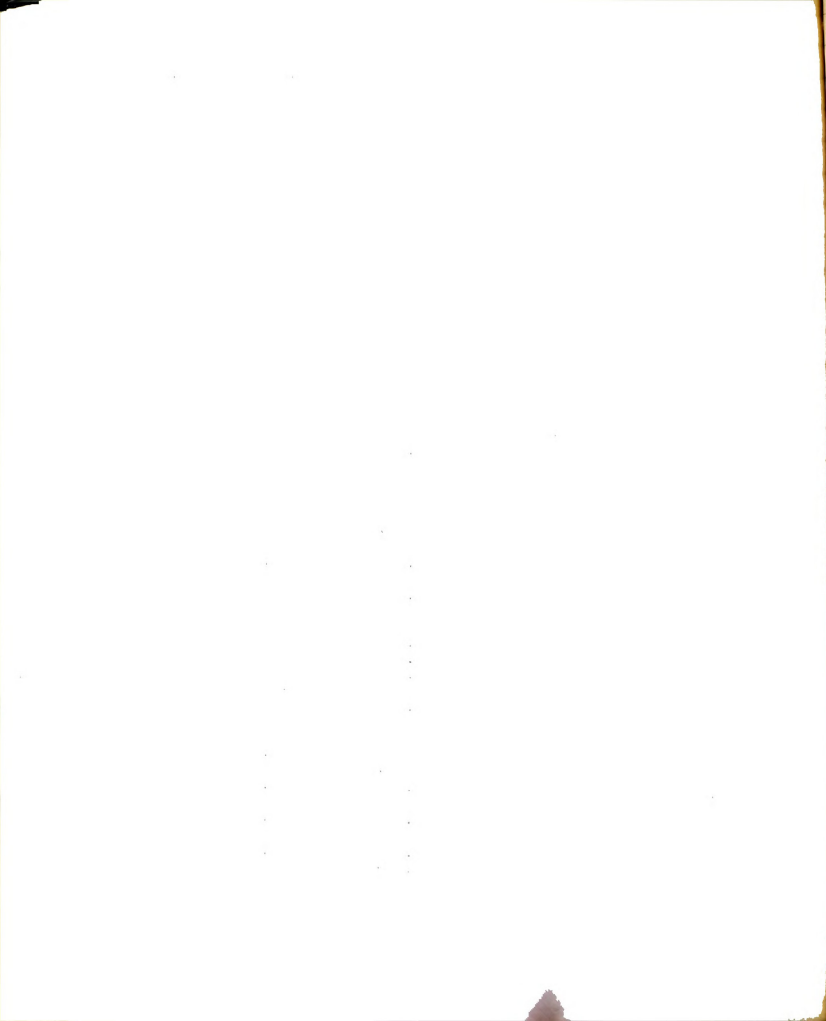
1-0	N40	PL	15/2-	1727,3000	1,96-004
1-0	N40	PL	15/2	1727,4000	3,92-004
1-0	N40	PL	15/2+	1727,4000	1,96-004
1-0	N40	PL	17/2-	1723,0000	1,82-004
1-0	N40	PL	17/2+	1723,0000	1,82-004
1-0	N40	PL	19/2-	1718,4000	1,65-004
1-0	N40	PL	19/2+	1718,5000	1,65-004
1-0	N40	PL	21/2-	1713,8000	1,46-004
1-0	N40	PL	21/2+	1713,9000	1,46-004
1-0	N40	PL	23/2-	1709,0000	1,26-004
1-0	N40	PL	23/2+	1709,1000	1,26-004
1-0	N40	PL	25/2-	1704,1000	1,06-004
1-0	N40	PL	25/2+	1704,3000	1,06-004
1-0	N40	PL	29/2-	1694,1000	6,98-005
1-0	N40	PL	29/2+	1694,2000	6,98-005
1-0	N40	PL	31/2-	1688,9000	5,49-005
1-0	N40	PL	31/2+	1689,0000	5,49-005
1-0	N40	PL	33/2-	1683,5000	4,22-005
1-0	N40	PL	33/2+	1683,7000	4,22-005
1-0	N40	PL	35/2-	1678,1000	3,18-005
1-0	N40	PL	35/2+	1678,3000	3,18-005
1-0	N40	QL	3/2	1756,1000	2,41-004
1-0	N40	QL	7/2	1755,3000	5,16-004
1-0	N40	QL	9/2	1754,7000	6,06-004
1-0	N40	QL	11/2+	1754,0000	3,33-004
1-0	N40	QL	13/2-	1753,1000	3,47-004
1-0	N40	QL	13/2	1753,2000	6,95-004
1-0	N40	QL	13/2+	1753,2000	3,47-004
1-0	N40	QL	15/2	1752,2000	6,97-004
1-0	N40	QL	17/2	1751,1000	6,75-004
1-0	N40	QL	19/2-	1749,8000	3,17-004
1-0	N40	QL	21/2-	1748,5000	2,90-004
1-0	N40	QL	21/2+	1748,6000	2,90-004
1-0	N40	QL	23/2-	1747,0000	2,58-004
1-0	N40	QL	23/2+	1747,2000	2,58-004
1-0	N40	RL	7/2-	1770,2000	9,06-005
1-0	N40	RL	7/2+	1770,2000	9,06-005
1-0	N40	RL	11/2-	1775,5000	1,30-004
1-0	N40	RL	17/2-	1782,5000	1,39-004
1-0	N40	RL	17/2+	1782,6000	1,39-004
1-0	N40	RL	21/2-	1786,6000	1,20-004
1-0	N40	RL	21/2+	1786,7000	1,20-004
1-0	N40	RL	27/2-	1791,8000	7,79-005
1-0	N40	RL	27/2+	1791,9000	7,79-005
1-0	N40	RL	29/2-	1793,3000	6,40-005
1-0	N40	RL	29/2+	1793,5000	6,40-005



APPENDIX V-A

G-FACTORS FOR $^{14}\text{N}16\text{O}$

SUBSTATE	J	VALUES	
		V=0	V=1
1	1/2	0,0000	0,0000
1	3/2	0,0230	0,0228
1	5/2	0,0263	0,0260
1	7/2	0,0273	0,0270
1	9/2	0,0277	0,0274
1	11/2	0,0279	0,0276
1	13/2	0,0279	0,0276
1	15/2	0,0278	0,0275
1	17/2	0,0277	0,0274
1	19/2	0,0276	0,0273
1	21/2	0,0274	0,0271
1	23/2	0,0272	0,0269
1	25/2	0,0270	0,0267
1	27/2	0,0267	0,0265
1	29/2	0,0265	0,0262
1	31/2	0,0262	0,0260
1	33/2	0,0259	0,0257
1	35/2	0,0256	0,0254
1	37/2	0,0253	0,0251
1	39/2	0,0250	0,0248
1	41/2	0,0247	0,0245
1	43/2	0,0244	0,0242
1	45/2	0,0241	0,0239
1	47/2	0,0238	0,0236
1	49/2	0,0235	0,0233
1	51/2	0,0232	0,0230
2	3/2	0,7770	0,7772
2	5/2	0,3166	0,3168
2	7/2	0,1632	0,1635
2	9/2	0,0935	0,0938
2	11/2	0,0561	0,0564
2	13/2	0,0337	0,0340
2	15/2	0,0192	0,0195
2	17/2	0,0095	0,0097
2	19/2	0,0025	0,0028

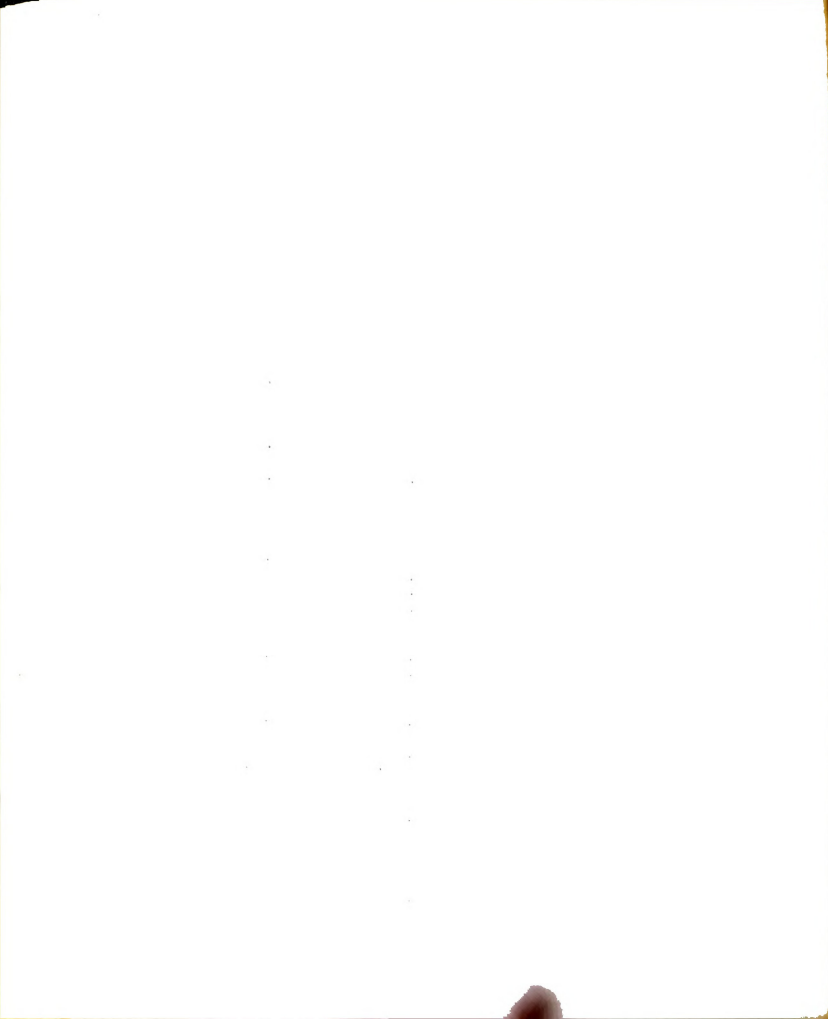


2	21/2	-0,0025	-0,0023
2	23/2	-0,0063	-0,0060
2	25/2	-0,0092	-0,0089
2	27/2	-0,0114	-0,0111
2	29/2	-0,0131	-0,0129
2	31/2	-0,0145	-0,0142
2	33/2	-0,0155	-0,0153
2	35/2	-0,0164	-0,0161
2	37/2	-0,0170	-0,0168
2	39/2	-0,0175	-0,0173
2	41/2	-0,0179	-0,0177
2	43/2	-0,0182	-0,0180
2	45/2	-0,0184	-0,0183
2	47/2	-0,0186	-0,0184
2	49/2	-0,0187	-0,0185
2	51/2	-0,0187	-0,0186

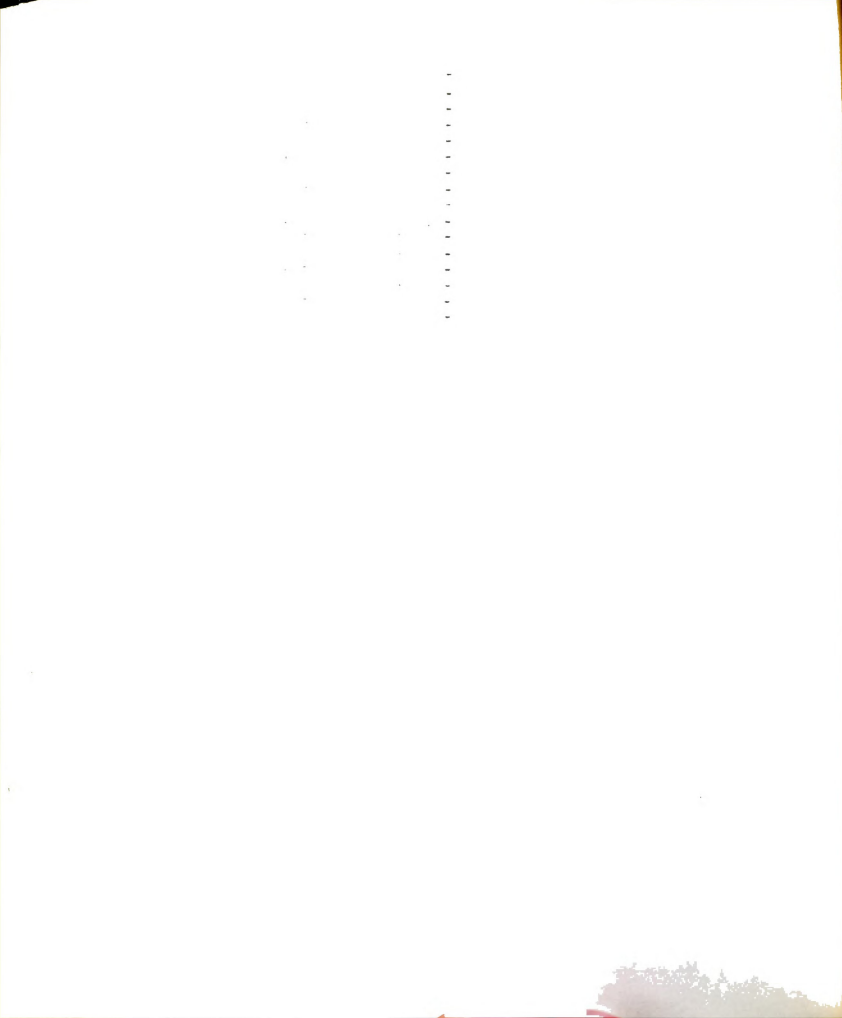
APPENDIX V-B

G-FACTORS FOR $^{15}\text{N}16\text{O}$

SUBSTATE	J	VALUES	
		V=0	V=1
1	1/2	0,0000	0,0000
1	3/2	0,0221	0,0228
1	5/2	0,0252	0,0260
1	7/2	0,0262	0,0270
1	9/2	0,0266	0,0274
1	11/2	0,0268	0,0275
1	13/2	0,0268	0,0276
1	15/2	0,0267	0,0275
1	17/2	0,0266	0,0274
1	19/2	0,0265	0,0272
1	21/2	0,0264	0,0271
1	23/2	0,0262	0,0269
1	25/2	0,0260	0,0267
1	27/2	0,0258	0,0264
1	29/2	0,0255	0,0262
1	31/2	0,0253	0,0259
1	33/2	0,0251	0,0257
1	35/2	0,0248	0,0254
1	37/2	0,0245	0,0251
1	39/2	0,0243	0,0248
1	41/2	0,0240	0,0245
1	43/2	0,0237	0,0242
1	45/2	0,0234	0,0239
1	47/2	0,0231	0,0236
1	49/2	0,0228	0,0233
1	51/2	0,0226	0,0230
2	3/2	0,7779	0,7772
2	5/2	0,3176	0,3169
2	7/2	0,1643	0,1635
2	9/2	0,0946	0,0938
2	11/2	0,0572	0,0564
2	13/2	0,0348	0,0340
2	15/2	0,0203	0,0196
2	17/2	0,0105	0,0098
2	19/2	0,0036	0,0028



2	21/2	-0,0015	-0,0022
2	23/2	-0,0053	-0,0060
2	25/2	-0,0082	-0,0089
2	27/2	-0,0104	-0,0111
2	29/2	-0,0122	-0,0128
2	31/2	-0,0136	-0,0142
2	33/2	-0,0147	-0,0153
2	35/2	-0,0155	-0,0161
2	37/2	-0,0162	-0,0168
2	39/2	-0,0168	-0,0173
2	41/2	-0,0172	-0,0177
2	43/2	-0,0175	-0,0180
2	45/2	-0,0177	-0,0182
2	47/2	-0,0179	-0,0184
2	49/2	-0,0180	-0,0185
2	51/2	-0,0181	-0,0186



APPENDIX VI

The expressions used in the combination difference, frequency and Λ -splitting fits are as follows:

A) Combination differences

$$\begin{aligned}
 \Delta_n F^i(J, v) = & [U(J+n) - U(J)] \times B_{0i} \\
 & - [U(J+n)^2 - U(J)^2] \times D_{0i} \\
 & + (-1)^i [U(J+n)^3 - U(J)^3] \times H_0 \\
 & - [U(J+n) - U(J)] v \times \alpha_i \\
 & - [U(J+n)^2 - U(J)^2] v \times \beta_i \\
 & - (-1)^i [U(J+n)^3 - U(J)^3] v \times \gamma' ,
 \end{aligned}$$

where $i = 1, 2$ refers to the $^2\Pi_1$ and $^2\Pi_2$ states respectively, $n = 1, 2$ corresponding to a difference of 1, 2 in J respectively and $U(J) = (J + \frac{1}{2})^2$.

B) Frequencies

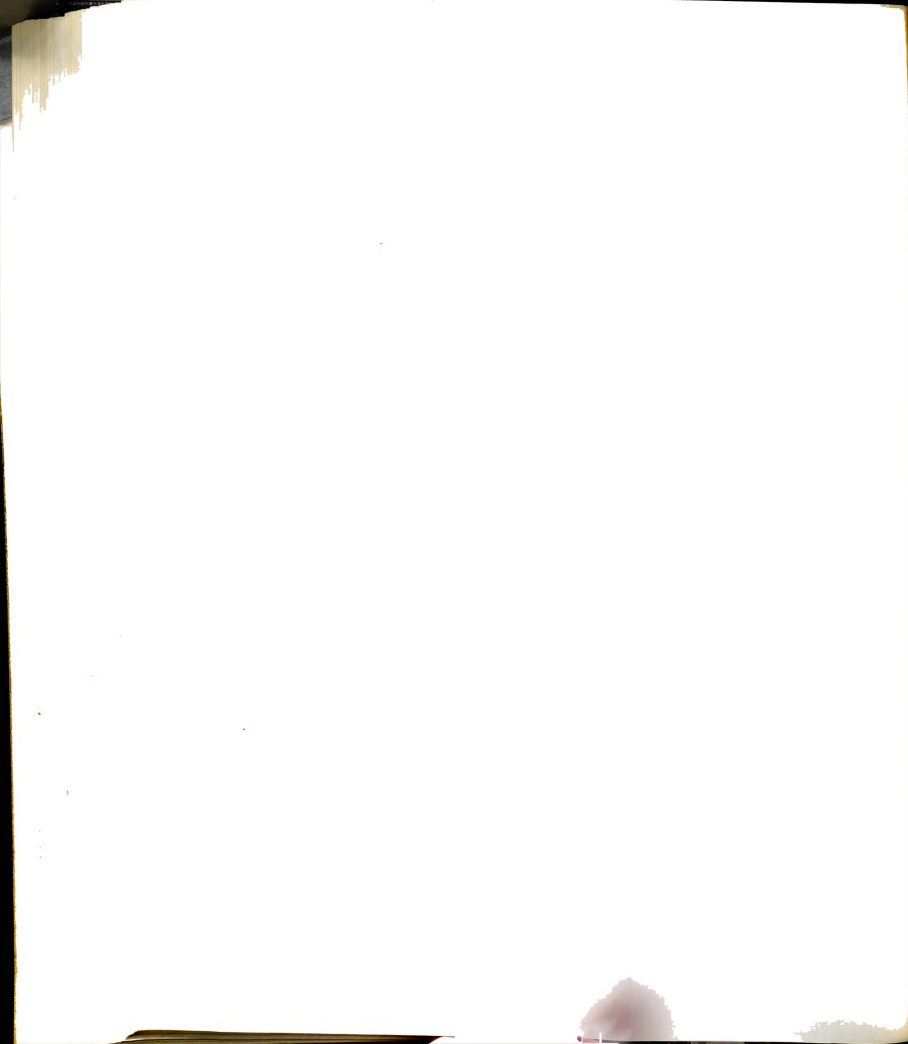
$$\begin{aligned}
 v(J, n, v, s) = & 1.0 \times \Delta G(1) \\
 & + (\delta_{H,s} - \delta_{L,s}) \times Q_0 \\
 & + (\delta_{1,s} - \delta_{2,s} - \delta_{H,s} + \delta_{L,s}) v/2 \times X \\
 & + \{ [U(J+n) - U(J)] \delta_{1,s} - U(J) \delta_{H,s} + U(J+n) \delta_{L,s} \} \times B_{01} \\
 & + \{ [U(J+n) - U(J)] \delta_{2,s} + U(J+n) \delta_{H,s} - U(J) \delta_{L,s} \} \times B_{02}
 \end{aligned}$$



(cont.)

$$\begin{aligned}
& - \{ [U(J+n)^2 - U(J)^2] \delta_{1,s} - U(J)^2 \delta_{H,s} + U(J+n)^2 \delta_{L,s} \} \quad \times \quad D_{01} \\
& - \{ [U(J+n)^2 - U(J)^2] \delta_{2,s} + U(J+n)^2 \delta_{H,s} - U(J)^2 \delta_{L,s} \} \quad \times \quad D_{02} \\
& - \{ [U(J+n)^3 - U(J)^3] \delta_{1,s} - U(J)^3 \delta_{H,s} + U(J+n)^3 \delta_{L,s} \} \quad \times \quad H_0^1 \\
& + \{ [U(J+n)^3 - U(J)^3] \delta_{2,s} + U(J+n)^3 \delta_{H,s} - U(J)^3 \delta_{L,s} \} \quad \times \quad H_0^1 \\
& - \{ [U(J+n) + \frac{1}{2}] (\delta_{1,s} + \delta_{L,s}) - \frac{1}{2} (\delta_{2,s} + \delta_{H,s}) \} v \quad \times \quad \alpha_1 \\
& - \{ [U(J+n) - \frac{1}{2}] (\delta_{2,s} + \delta_{H,s}) + \frac{1}{2} (\delta_{1,s} + \delta_{L,s}) \} v \quad \times \quad \alpha_2 \\
& - \{ [U(J+n)^2 + \frac{1}{2}] (\delta_{1,s} + \delta_{L,s}) + \frac{1}{2} (\delta_{2,s} + \delta_{H,s}) \} v \quad \times \quad \beta_1 \\
& - \{ [U(J+n)^2 + \frac{1}{2}] (\delta_{2,s} + \delta_{H,s}) + \frac{1}{2} (\delta_{1,s} + \delta_{L,s}) \} v \quad \times \quad \beta_2 \\
& \quad + \quad [U(J+n)^3] v (\delta_{1,s} + \delta_{L,s}) \quad \times \quad \gamma' \\
& \quad - \quad [U(J+n)^3] v (\delta_{2,s} + \delta_{H,s}) \quad \times \quad \gamma' ,
\end{aligned}$$

$U(J)$ is the same as for the combination differences except that $n = -1, 0, +1$ corresponding to the P, Q, and R branches respectively, and $\delta_{1,s}$, $\delta_{2,s}$, $\delta_{H,s}$, and $\delta_{L,s}$ are Kronecker deltas having the value 1 or 0 depending upon whether s is equal or unequal to the other subscript. The 1, 2, H, and L refer to the ${}^2\Pi_{1/2}$, ${}^2\Pi_{3/2}$ subbands, the HES and LES respectively.



C) Λ -splitting expressions

$$U(J) = (J^2 - \frac{1}{4})(J + \frac{3}{2})$$

$$F(J) = (J + \frac{1}{2})$$

1-subband

$$\begin{aligned} \Delta v(J-1; J) &= 2\{1 + U(J-1)[\lambda_{11}-2]^{-2} + U(J)[\lambda_{01}-2]^{-2}\}p_{\Lambda} \\ &\quad + 4\{U(J-1)[\lambda_{11}-2]^{-1} + U(J)[\lambda_{01}-2]^{-1}\}q_{\Lambda} \end{aligned}$$

$$\begin{aligned} -\Delta v(J; J) &= -2\{2F(J) - U(J)[\lambda_{11}-2]^{-2} - U(J)[\lambda_{01}-2]^{-2}\}p_{\Lambda} \\ &\quad + 4U(J)\{[\lambda_{11}-2]^{-1} + [\lambda_{01}-2]^{-1}\}q_{\Lambda} \end{aligned}$$

$$\begin{aligned} -\Delta v(J+1; J) &= -2\{1 - U(J+1)[\lambda_{11}-2]^{-2} + U(J)[\lambda_{01}-2]^{-2}\}p_{\Lambda} \\ &\quad + 4\{U(J+1)[\lambda_{11}-2]^{-1} - U(J)[\lambda_{01}-2]^{-1}\}q_{\Lambda} \end{aligned}$$

2-subband

$$\begin{aligned} \Delta v(J-1; J) &= 2\{U(J)[\lambda_{02}-2]^{-2} - U(J-1)[\lambda_{12}-2]^{-2}\}p_{\Lambda} \\ &\quad + 4\{U(J)[\lambda_{02}-2]^{-1} - U(J-1)[\lambda_{12}-2]^{-1}\}q_{\Lambda} \end{aligned}$$

$$\begin{aligned} -\Delta v(J; J) &= -2U(J)\{[\lambda_{02}-2]^{-2} + [\lambda_{12}-2]^{-2}\}p_{\Lambda} \\ &\quad - 4U(J)\{[\lambda_{02}-2]^{-1} + [\lambda_{12}-2]^{-1}\}q_{\Lambda} \end{aligned}$$

$$\begin{aligned} -\Delta v(J+1; J) &= 2\{U(J)[\lambda_{02}-2]^{-2} - U(J+1)[\lambda_{12}-2]^{-2}\}p_{\Lambda} \\ &\quad + 4\{U(J)[\lambda_{02}-2]^{-1} - U(J+1)[\lambda_{12}-2]^{-1}\}q_{\Lambda} \end{aligned}$$



HES

$$\begin{aligned}\Delta v(J-1;J) &= 2\{F(J) - U(J-1)[\lambda_{12}-2]^{-2} - U(J)[\lambda_{01}-2]^{-2}\}p_{\Lambda} \\ &\quad - 4\{U(J)[\lambda_{01}-2]^{-1} + U(J-1)[\lambda_{12}-2]^{-1}\}q_{\Lambda}\end{aligned}$$

$$\begin{aligned}-\Delta v(J;J) &= -2\{F(J) + U(J)[\lambda_{12}-2]^{-2} - U(J)[\lambda_{01}-2]^{-2}\}p_{\Lambda} \\ &\quad - 4 U(J)\{[\lambda_{12}-2]^{-2} - [\lambda_{01}-2]^{-1}\}q_{\Lambda}\end{aligned}$$

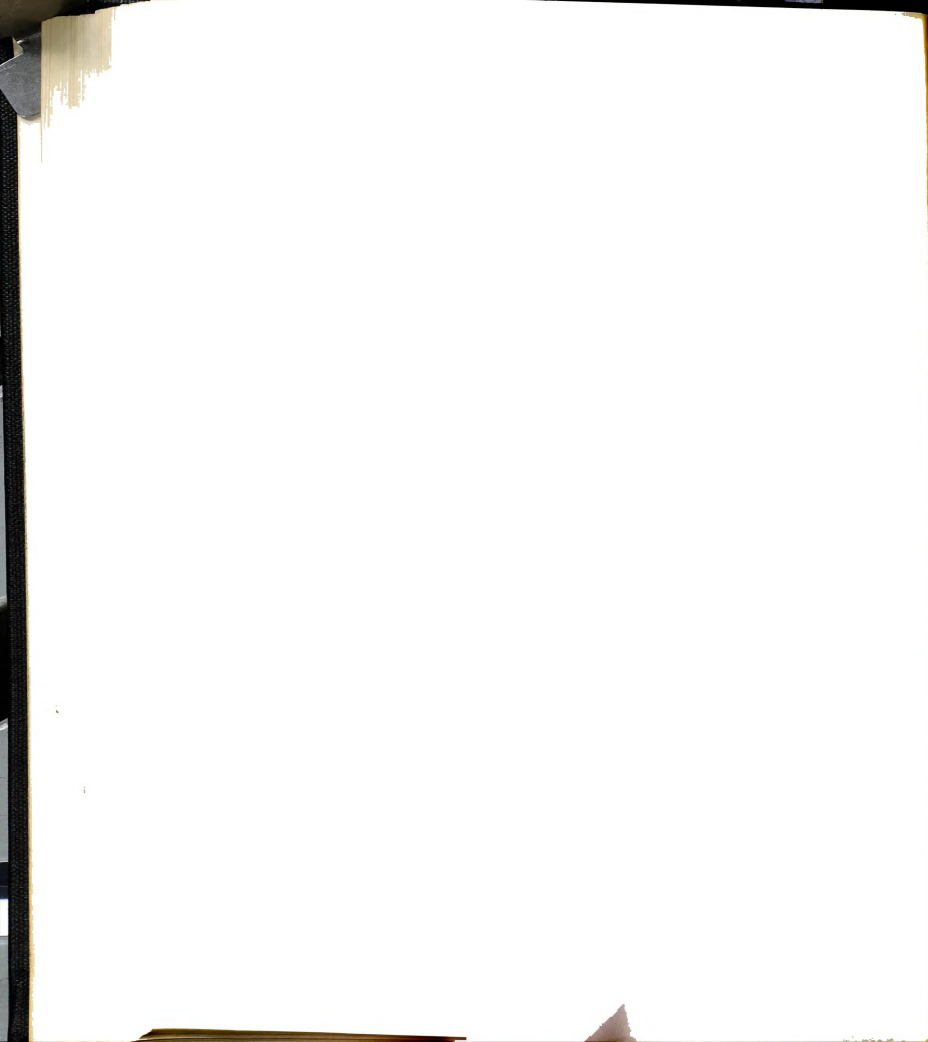
$$\begin{aligned}\Delta v(J+1;J) &= 2\{F(J) - U(J+1)[\lambda_{12}-2]^{-2} - U(J)[\lambda_{01}-2]^{-2}\}p_{\Lambda} \\ &\quad -4\{U(J+1)[\lambda_{12}-2]^{-1} + U(J)[\lambda_{01}-2]^{-1}\}q_{\Lambda}\end{aligned}$$

LES

$$\begin{aligned}-\Delta v(J-1;J) &= -2\{F(J) - U(J-1)[\lambda_{11}-2]^{-2} - U(J)[\lambda_{02}-2]^{-2}\}p_{\Lambda} \\ &\quad + 4\{U(J-1)[\lambda_{11}-2]^{-1} + U(J)[\lambda_{02}-2]^{-1}\}q_{\Lambda}\end{aligned}$$

$$\begin{aligned}-\Delta v(J;J) &= -2\{F(J) + U(J)[\lambda_{02}-2]^{-2} - U(J)[\lambda_{11}-2]^{-2}\}p_{\Lambda} \\ &\quad + 4 U(J)\{[\lambda_{11}-2]^{-1} - [\lambda_{02}-2]^{-1}\}q_{\Lambda}\end{aligned}$$

$$\begin{aligned}-\Delta v(J+1;J) &= -2\{F(J) - U(J+1)[\lambda_{11}-2]^{-2} - U(J)[\lambda_{02}-2]^{-2}\}p_{\Lambda} \\ &\quad + 4\{U(J+1)[\lambda_{11}-2]^{-1} + U(J)[\lambda_{02}-2]^{-1}\}q_{\Lambda}\end{aligned}$$



APPENDIX VII

COMPUTER PROGRAMS

Many computer programs were written during the course of this work. The major ones are described below with operating instructions.

A. SHAFT

This intricate and very useful program written by L. E. Bullock is designed to reduce the raw data, including code weights from up to eight separate Hydrel measurements of a band to a tabulated output of the average fringe number, weighted average frequency, weighted standard deviation, individual measurements and weights of each line measured in the band. It will also identify these lines. SCAN and CALFIT (written by M. D. Olman (74)) are used as subroutines. SCAN determines the fringe numbers of the individual lines including calibration lines. Standard calibration frequency decks are input and matched with the observed calibration lines. CALFIT performs a least squares fit of the calibration lines to determine the fringe constants which are then used to obtain frequencies for the observed lines. The frequencies are ordered and a weighted average of identical transitions is performed. All this information is tabulated

in a convenient output which includes identification of the transitions, if this is known. This program can also be used like a normal SCAN program with the option of getting punched output of the frequencies, which can later be used in place of the raw Hydell data to obtain the tabulated output. The user provides the program with identification decks and a series of tolerances which indicate his maximum uncertainty in the frequency (in cm^{-1}) of any line so that the program is able to recognize separate measurements of the same line. All tolerances and other quantities necessary for operation are preset to typical values which will be used in the event they are omitted on input.

STRUCTURE OF DATA DECK

I. Option card

<u>Col.</u>	<u>Variable</u>	<u>Field</u>	<u>Function</u>
1	NGPS	I	Indicates number of groups ≤ 8 to be averaged.
2	IOP(1)	I	$\neq 0$ indicates SCAN desired (see SCAN description for input).
3	IOP(2)	I	$\neq 0$ indicates average desired. =2 indicates punch of identification, average frequency and weight in the identification deck format is desired.
4	IOP(3)	I	$\neq 0$ indicates punch frequencies and weights (8/card) is desired from SCAN.
5	IDNT	I	$\neq 0$ identification deck(s) is used. =2 identification deck(s) is input.



<u>Col.</u>	<u>Variable</u>	<u>Field</u>	<u>Function</u>
6	ICAL	I	≠0 calibration deck(s) is used. =2 calibration deck(s) is input. =3 causes fringe constants just determined to be used to obtain line frequencies (see below).
7	IDON	I	=1 provides printout of single frequencies in the "group" tabulation. =2 omits punching weights as provided in IOP(2)=2.
11-20	TOL1	F	Frequencies within a group which differ by less than TOL1 are considered to be separate measurements of one line, and their non-weighted average is formed. TOL1 is preset to 0.05.
21-30	TOL2	F	Frequencies in the various groups which differ by less than TOL2 are considered to be measurements of the same line. TOL2 is preset to TOL1.
31-40	TOL3	F	Frequencies which differ by less than TOL3 from input identification frequencies are assigned the corresponding identification. If two identifications within TOL3 are found, an asterisk field is printed. If TOL3 is greater than 100 the asterisk field is suppressed and the same identification may be punched and/or printed for all lines.

II. IDENTIFY data deck

This section handles both identification and calibration decks and appears if and only if IDNT or ICAL are equal to 2.

1. Order card: This card is used to convert input frequencies from their value in the order in which they were recorded to their value in the order of the IR. It can be inserted anywhere in the identification deck.



<u>Col.</u>	<u>Variable</u>	<u>Field</u>	<u>Function</u>
8	IR	I	Order in which the IR radiation was recorded.
16	IICAL	I	Order in which the identification or calibration line would have been or was recorded.
75-80	ORDER	A	"ORDER" specifies an ORDER card.

(Note: if the ORDER card does not appear IR and IICAL are assumed to be one.)

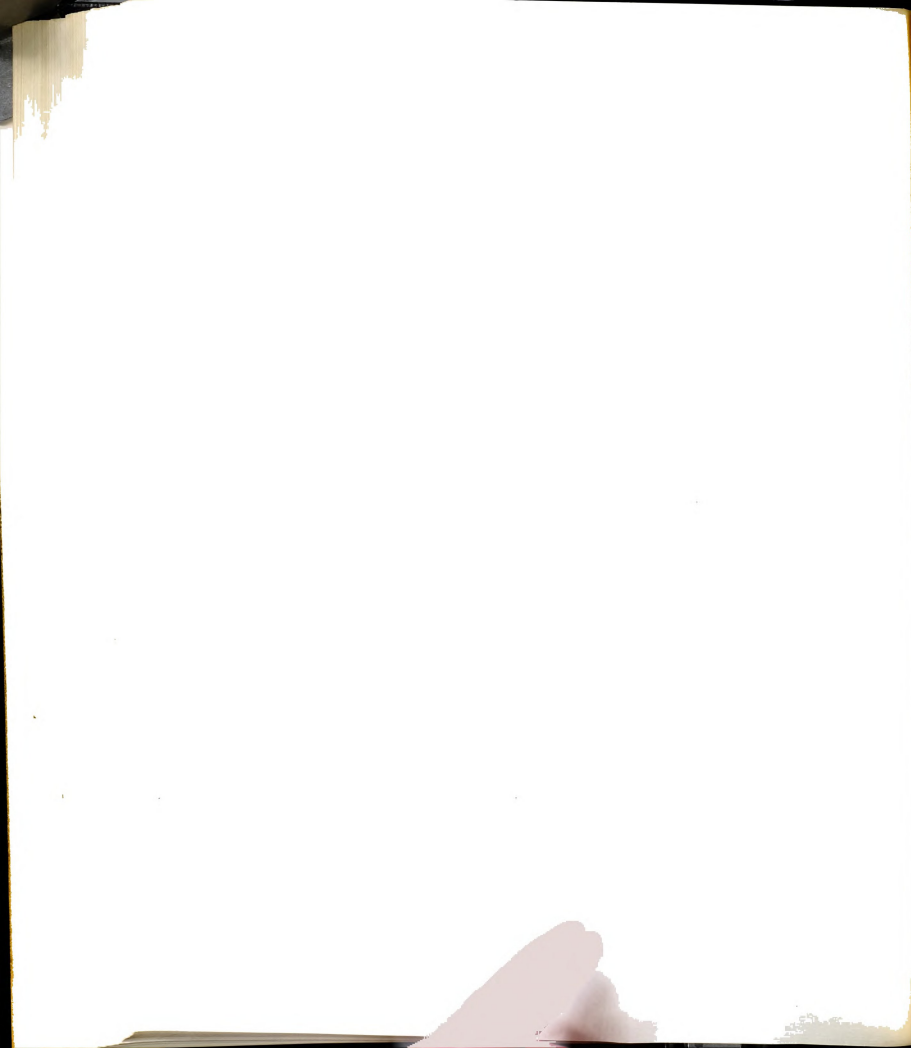
2. Ident deck cards:

1-8	NAME1	A	These two fields contain the identification title that is desired to be printed and/or punched beside the corresponding frequency.
9-16	NAME2	A	
20-33	XNU	F	Frequency of identification or calibration line.

These cards are read until a value of XNU=0 is encountered.

III. SCAN data deck

This section appears if and only if IOP(1) $\neq$ 0. A description of the SCAN deck is given elsewhere. (The basic structure is: NEW SCAN card, operator name card, heading cards, calibration constants card (option), Hydel cards, and 8- or 9-parameter card.) A non-zero punch in cols. 23-27 of a 1-parameter card acts as a switch to either begin or end punch/averaging depending upon whether the switch was on or off before. If punch frequencies are obtained, the fringe constants used are also punched, whenever they are set, and included with the frequencies. This is done in a format recognized in the averaging section. The first NGPS groups must end with an 8-parameter card. The last group ends with a 9-parameter card. The



punch/averaging switch is off at the start of each group.

IV. AVFRQ (averaging) data deck

1. Heading cards: Cols. 1-72 of these cards will be listed on the output. This will continue until END HEAD is found in cols. 73-80. Cols. 1-72 of the last card will also appear as a heading for the output of each page of this set of data. If IDNT $\neq$ 0 and the word "IDN HEAD" appears in cols. 73-80, the first 32 cols. of this card are used as a two line column heading over the identification titles. If this card does not appear, the word IDENTIFICATION is used. (Read by 10A8)

2. Group identification and data (appears NGPS times):

Cards a,c must appear once and only once for each group.

Cards b, d, e, and f may appear as many times as needed.

Up to $(10000/\text{NGPS}+1)$ data points may appear in each group.

a) Column heading card: Contains column headings for the tabulated output of individual measurements. Place the first line of heading in cols. 1-8, the second line in cols. 9-16. If non-zero numbers are found in cols. 21-35 and 36-50 they are treated as updated values of the fringe constants A and B respectively. These numbers are used to convert all succeeding frequencies in this group, and a new set of punch frequencies is given.

b) Punched frequency cards: Frequencies and weights punched from SCAN or a previous run may be entered here. The format is 8(4PF8,R1,X). Frequencies and weights



are read from left to right across the card until the first three fields are zero.

i) If the first field is zero, the card is treated as a fringe constants card. The last value read is used in fringe number calculations. Values may be input; A in cols. 16-19 and 21-25, and B in cols. 35-39 and 40-44. No decimal point is used!!

ii) If the first two fields are zero, the card is treated as a code-weight specification card. If this card does appear the codes weights are read; 4, cols. 21-28; 3, cols. 31-38; 2, cols. 41-48; 1, cols. 51-58; blank, cols. 61-68. If this card does not appear the code weights are assigned: 4=1.0, 3=0.25, 2=0.62; 1=0.16; 0= 10^{-20} ; blank=1.0. The last code weight card is used to assign all code weights for that particular group.

c) Blank card: Card with first 20 columns blank to indicate the end of the punched data.

d) Delete cards: DELETE in cols. 11-16 with frequency to be deleted in cols. 21-35.

e) Change cards: CHANGE in cols. 11-16 with frequency to be changed in cols. 21-35, new/old value of frequency in cols. 36-50 and weight code in col. 52.

f) Punch card: PUNCH in cols. 12-16 causes average frequencies of this particular group, including changes and excluding deletes to be punched out in the normal format of b) above.

3. Calibration constants card: Fringe constant A in cols. 21-35, B in cols. 36-50. If this card is blank the last values of fringe constants will be used.

V. SEARCH data deck

This section appears if ICAL $\neq$ 0 and must be used in conjunction with the averaging section. Its purpose is to match SCAN fringe numbers with the corresponding calibration frequencies and finally do a least squares fit to determine the fringe constants. A punch deck of the assigned fringe numbers, frequencies and weights is punched out in the standard CALFIT format.

1. Number of lines card: This card specifies the number of calibration line fringe numbers input from SCAN; cols. 1-10. The search is carried out twice unless the number of lines identified equals or exceeds the number of lines on this card on the first pass.

2. Initial identification cards: At least two initial identifications of calibration lines must be made and input. This input consists of the identification title exactly as it was read in for the calibration deck, and the approximate fringe number (within one) of the calibration line. The identification is put in cols. 1-16 (A-format) and the fringe number is in cols. 30-39.

3) Blank card: A blank card signals the end of initial identification cards.



4. Heading cards: These are heading cards for the CALFIT subroutine. Cols. 1-72 of the cards are read and printed until a card with END HEAD in cols. 73-80 is encountered. The last card is repeated at the top of all succeeding pages.

VI. New case

NEW CASE in cols. 73-80 indicates that a new case beginning with the option card follows. Note that if the fringe constants just determined in section V are to be used for new SCAN data, a new case is called for with ICAL=3.

VII. Stop card

STOP in cols. 77-80 ends execution of the program.

A listing of the program follows.



```

FILE,69
MAIN,5
FILE END
FTN,L,X
      PROGRAM SHAFT
C  SCAN HYDEL AVERAGE FREQUENCIES TABULATE
COMMON/1/IOP(3),ILS(3),TOL1,TOL2,TOL3,A,B,LP,IDNT,ICAL,IDON,JUMP
COMMON/2/ N
COMMON/3/NAME1(2000),NAME2(2000),NU(2000),NMAX
COMMON/8/ICHEAD(9),IHEAD(9,2),IDN(4)
COMMON/5/AVGFREQ(200),AWGT(200),NUM
COMMON/9/ CCWT(3,5)
DIMENSION FRQ(1,10000),WTS(1,10000)
TYPE INTEGER WIT,WT,WTS
1  READ 100,NGPS,IOP,IDNT,ICAL,IDON,TOL1,TOL2,TOL3,IFDONE
   IF(IFDONE, .EQ. 8H  STOP) STOP
   IDN(1)=8H          $ IDN(2)=8H          $ IDN(3)=8H
   IDN(4)=8H
   JUMP=0
   IDEM=10000./NGPS
   IF (IDNT.F0.2.0H,ICAL.EQ.2) CALL OVERLAY(1,,1,,)
   IF (IDNT) 8200,8100
8100 LP=1
      NAME1(1)=NAME2(1)=8H
8200 CONTINUE
      N=1
      DO 10 I=1,NGPS
10  ILS(I)=1
      IF(TOL1.EQ.0.) TOL1=.050
      IF(TOL2.EQ. 0.) TOL2=TOL1
      IF(TOL3.NE. 0.) GO TO 13
      IF(ICAL) TOL3=.03
      TOL3=.04-TOL3
13  IF(IOP(1)) CALL OVERLAY(2,,2,J,FRQ,WTS,NGPS,IDEM)
14  IF(IOP(2)) CALL OVERLAY(3,,3,J,FRQ,WTS,NGPS,IDEM)
      IF(ICAL) 16,200
16  CALL OVERLAY(4, ,4,,)
      JUMP=1
      ICAL=0
      IDNT=1
      GO TO 14
200 READ 160, IFDONE
      IF(IFDONE.EQ.8H          ) GO TO 200
      IF(IFDONE.EQ.8HEND HEAD) GO TO 200
      IF(IFDONE.EQ.8HNEW CASE) GO TO 1
      IF(IFDONE.EQ. 8H  STOP) STOP
100 FORMAT(7I1,3X,3F10.8,32X,A8)
160 FORMAT (72X,A8)
      END

FILE,69
OVERLAY,1,1
FILE END

```



FTN,L,X

```

PROGRAM IDENTIFY
COMMON/1/IOP(3),ILS(8),TOL1,TOL2,TOL3,A,B,LP,IDNT,ICAL,IDON,JUMP
COMMON/3/NAME1(2000),NAME2(2000),NU(2000),NMAX
TYPE REAL NU
TYPE INTEGER ORDER
N=1
NT=1
IR=ICAL=1
20 READ 1,INAME1,INAME2,XNU,ORDER
IF(ORDER.EQ,8H ORDER)10,15
10 IR=INAME1=8H 0
ICAL=INAME2=8H 0
GO TO 20
15 IF(XNU) 16,25
16 XNU=XNU*IR/ICAL
IF(N.EQ,1) GO TO 6
5 IF(NU(NT-1),LE,XNU) GO TO 6
NU(NT)=NU(NT-1) * NAME1(NT)=NAME1(NT-1) * NAME2(NT)=NAME2(NT-1)
NT=NT+1
IF(NT-1) 6,6,5
6 NU(NT)=XNU * NAME1(NT)=INAME1 * NAME2(NT)=INAME2
N=N+1 * NT=N * GO TO 20
25 NMAX=N-1
IF(TOL3.GT,100.) GO TO 26
NAME1(NMAX+1)=NAME2(NMAX+1)=NAME1(NMAX+2)=8H
NAME2(NMAX+2)= 8H ***
NU(NMAX+1)=0.0
RETURN
26 NAME1(NMAX+2)=NAME1(1)
NAME2(NMAX+2)=NAME2(1)
RETURN
1 FORMAT (2A8,3X,F13.4,40X,A8)
END

```

FILE,69

OVERLAY,2,2

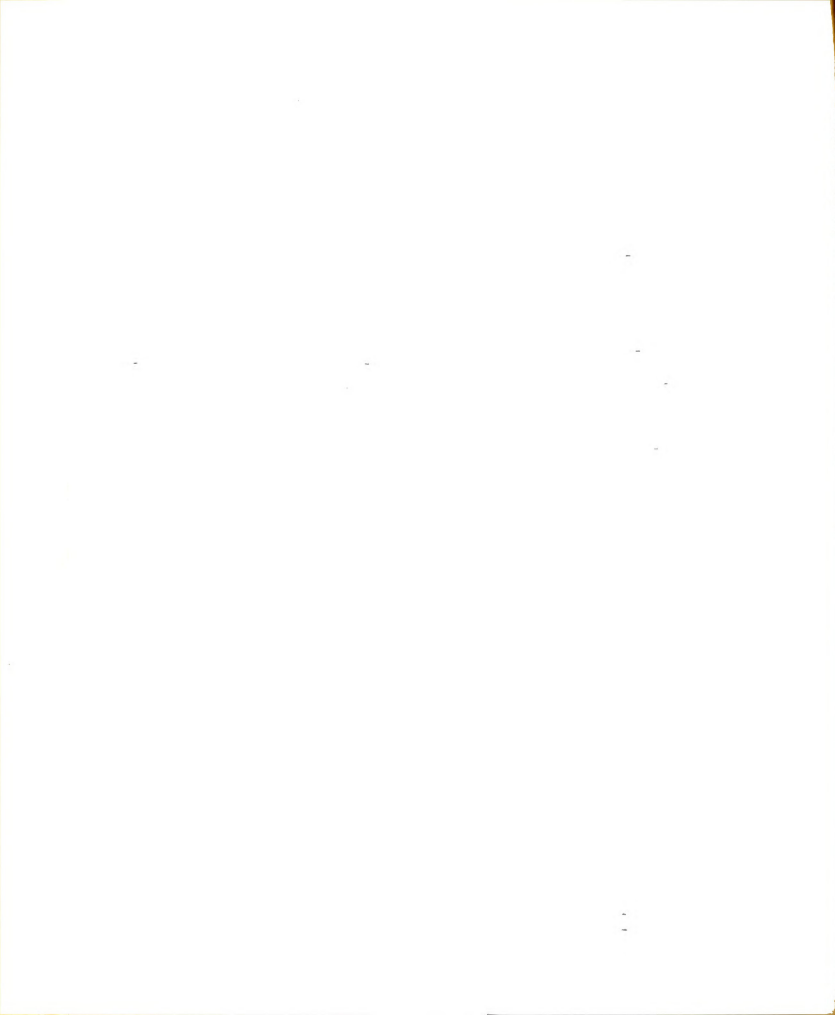
FILE END

FTN,L,X

```

PROGRAM ALL SCAN(FRQ,WTS,NGPS,IDEM)
COMMON/1/IOP(3),ILS(8),TOL1,TOL2,TOL3,A,B,LP,IDNT,ICAL,IDON,JUMP
COMMON/2/ NAVF
DIMENSION IFST(10),XM(6),YM(6),FRNGX(100),PSEP(100),FGSEP(100),
11I(2),I2(2),IHEAD(9),NAME(2),NHEAD(10),DELX(6),IPFR(3),IPEN(2),
2WT(6),WTT(8)
DIMENSION FRQ(NGPS,IDEM),WTS(NGPS,IDEM)
DATA(IPEN=8H6FIRST,8H6SECOND)
TYPE INTEGER WTT,WT,WTS
4 PRINT 9701
READ 7, NAME,IFDONE
7 FORMAT (2A8,56X,A8)
IF(IFDONE=8HNEW SCAN)11,13
11 IF(IFDONE=8HOLD SCAN)8,9

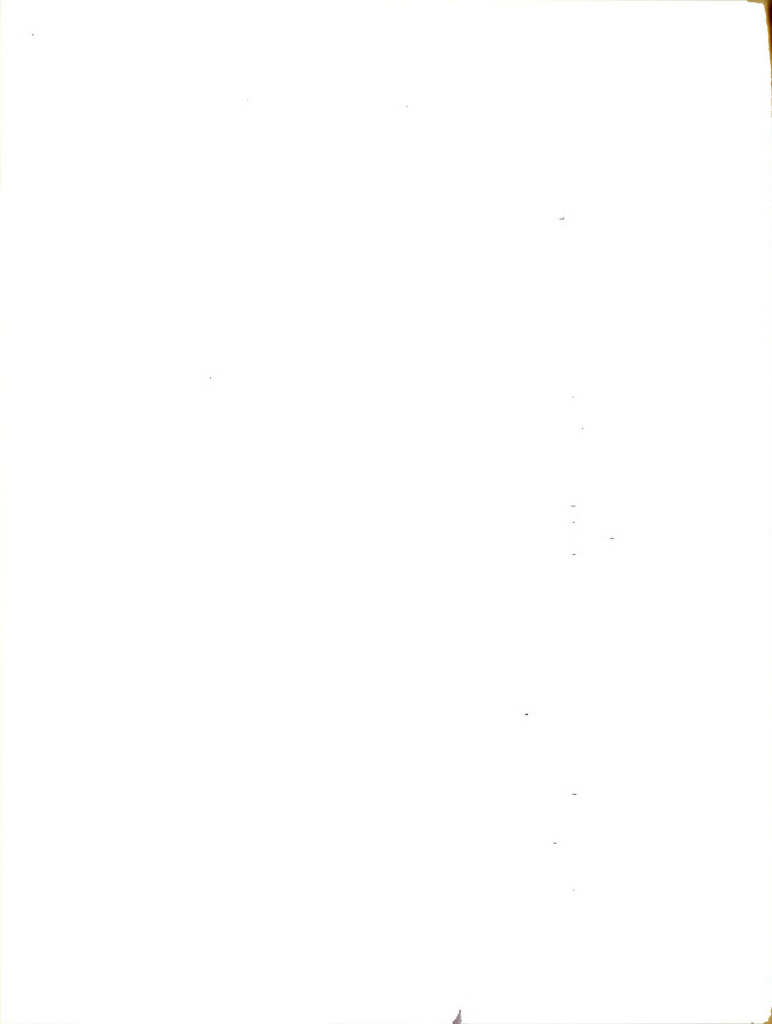
```




```

      8 PRINT 10
     10 FORMAT (81X*-NO NAME CARD-ASSUMING NEW SCAN*)
      GO TO 13
      9 INEW=0
      GO TO 1
     13 INEW=1
      1 READ 3, IHEAD, IFDONE
      PRINT 3, IHEAD
      IF (IFDONE=8) END HEAD) 1,2
      2 IH=NIP=1
      IF (IOP(3)) 9800,9900
9800 PUNCH 3, IHEAD
9900 CONTINUE
      NERM=NCAL=IP=ICARDS=IFRQQ=IPUNCH=0
      IH=ILT=IL=ILS(NAVF)=1
      MD=1
      XFSEP=FSEP=0.0
      ASSIGN 3600 TO NGO
      IF (ICAL) 334,335
     334 IF (ICAL .EQ. 3) GO TO 4001
      A=0.0 $ B=1.0 $ NCAL=1
      IF (.NOT. IOP(3)) GO TO 335
      JA=A $ IXA=(A-1A)*1,E5 $ IB=B*1,E5 $ XB=B*1,E5 $ IXB=(XB-IB)*1,E5
      PUNCH 70,IA,IXA,IB,IXB
     335 CONTINUE
     101 READ 100, (XM(I),YM(I),WT(I),I=1,6), ICODE, IFR
      IF (ICODE=6) 202,200,203
     203 IF (ICODE=8) 7000,8001,8001
     202 IF (4-ICODE) 5010,4000,204
     204 IF (ICODE=2) 205,2000,200
     205 IF (-ICODE) 1000,105,105
     105 PRINT 106, (XM(I),YM(I),I=1,6)
      GO TO 101
     102 PRINT 9701
      IF (ICAL .EQ. 3) ICAL=0
      RETURN
     200 NCOORD=6
      IF (XM(6)) 104,107
     107 DO 103 I=1,5
      NCOORD=NCOORD+1
     103 IF (XM(NCOORD)) GO TO 104
      GO TO 101
     104 DO 201 I=1,NCOORD
     201 XM(I)=OMT2*XM(I)-THETA*YM(I)
      IF (ICODE=5) 3000,5000,6000
1000 XFRN=XM
      XFRNG=YM
      FRNG=XFRNG-1.0
      IPP= XM(2)
      IF (IPUNCH) GO TO 411
      IPUNCH=XM(3)
      GO TO 410
     411 IF (XM(3)) IPUNCH=0
     410 CONTINUE

```



```

      GO TO 101
2000 SUMX=SUMY=SUMYY=SUMYX=0,0
      GO TO NGO
32  CONTINUE
      NOFR=0
      ASSIGN 6205 TO NIR
      DO 20 I = 1,6
      SUMY = SUMY + YM(I)
      SUMX = SUMX + XM(I)
      SUMYY = SUMYY + YM(I)*YM(I)
20  SUMYX = SUMYX + YM(I)*XM(I)
      THETA = (SUMYX - SUMY*SUMX/6,)/(SUMYY - SUMY*SUMY/6,)
      THETA2=0.5*THETA*THETA
      OMT2=1.0-THETA2
      IBAD = 0
      DO 30 I = 1,6
      DELX(I) = (SUMX-THETA*SUMY)/6. + THETA*YM(I) - XM(I)
      IF(ABS(DELX(I)),GT, 10.0) IBAD = 1
30  CONTINUE
      GO TO (101,31),IH
31  IF (,NOT, INEW) ENCODE(4,11,IFR) XFRM
      PRINT 9201,IHEAD,IFR,NAME
      IF(THETA2 ,GT, 0.0000125) PRINT 6210
      IF(IBAD) PRINT 6209
      GO TO 101
3000 DO3007J=2,NCOORD,2
      IP = IP + 1
      XFSEP=XFSEP+1,0
      PSEP(IP)=XM(J)-XM(J-1)
      FSEP=PSEP(IP)+FSEP
3007 CONTINUE
      GO TO 101
3600 NFRM=NFRM+1
      IPFR(NFRM)=IFR
      IF(,NOT, INEW) ENCODE(4,11,IPFR(NFRM))XFRM
11  FORMAT (F4)
      GO TO ( 32,3602),NFRM
3602 FSEP=FSEP/XFSEP
      N1=NFRM-1
      PRINT601,IPEN(N1),IPFR(N1),NAME ,THETA,DELX,(PSEP(I),I=NIP,IP)
601  FORMAT(A8*PEN SEPARATION FRAME IS NO,*A4/ * MEASURED BY *2A8/
1* ROTATION ANGLE IS*F10,6* RADIANS*/ * ROTATION FITS TO*6(F3*,*)* M
2ICHRONS*/ * OBSERVED PEN SEPARATIONS*(20F5))
3608 NIP=IP+1
      IF(THETA2 ,GT, 0.0000125) PRINT 6210
      IF(IBAD) PRINT 6209
      PRINT 3609,FSEP
3609 FORMAT (* AVERAGE PEN SEPARATION FOR THIS FRAME IS*F6,1* MICRONS*)
      FSEP=XFSEP=0.0
      IF(NFRM,EQ,2) GO TO 32
      IH=2
      ASSIGN 32 TO NGO
      PSFPSUM = 0
      DO 3701 J=1,IP

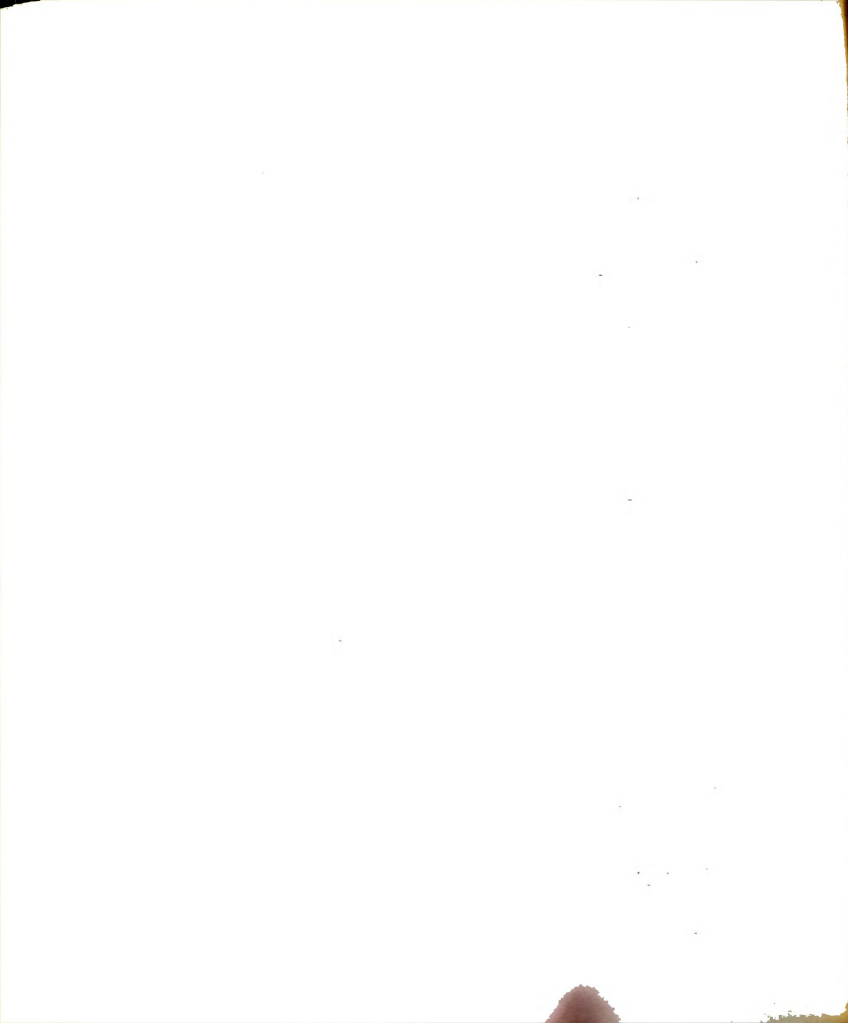
```



```

3701 PSEPSUM=PSEPSUM+PSEP(J)
      PENSEP = PSEPSUM/ IP
      PRINT 9300,PENSEP
      GO TO 32
4000 CONTINUE
      A = YM(1) + XM(2)*0.00001
      B=XM(3)+YM(3)*0.00001
      IF(YM(2) ,LT. 0.0) B=-B
      B=YM(2)+B*0.00001
4001 PRINT 9400, A, B
      NCAL=1
      IF(.NOT.IOP(3)) GO TO 101
      IA=A $ IXA=(A-IA)*1,E5 $ IR=B*1,E5 $ XB=B*1,E5 $ IXB=(XB-IB)*1,E5
      IF(IL,EQ,1) 71,8000
71 PUNCH 70,IA,IXA,IB,IXB
70 FORMAT(15X,14,X,15,8X,16,X,15)
      GO TO 101
5000 DO 5001 J = 1, NCOORD
      NOFR = NOFR + 1
      FRNGX(NOFR) = XM(J)
      FGSEP(NOFR)=FRNGX(NOFR)-FRNGX(NOFR-1)
5001 CONTINUE
      GO TO 101
5010 IF(NOFR) GO TO 200
      IF(.NOT,INEW) GO TO 200
      XFRNG=XM
      FRNG=XFRNG-1.0
      DO 5011 I=1,5
      XM(I)=XM(I+1)
5011 YM(I)=YM(I+1)
      XM(6)=YM(6)=0.0
      GO TO 200
6000 GO TO NIR
6205 PRINT 9500,XFRNG,THETA,DELX,(FGSEP(I),I=2,NOFR)
      ASSIGN 6204 TO NIR
      AVESEP=0.1*(FR NGX(NOFR)-FRNGX(1))/(NOFR-1.)
      IBAD = 0
      DO 6206 I=3,NOFR
6206 IF(ARSF(FGSEP(I)-FGSEP(I-1)) ,GT, AVESEP) IBAD = 1
      IF(IBAD) PRINT 6208
      M=0
      IF(NCAL) PRINT 9650,A,B
      PRINT 9655
      IF(IOP(3) ,AND, IPUNCH) PRINT 303
303 FORMAT (1H+,40X*THESE FREQUENCIES ARE BEING PUNCHED*)
6204 DO 6001 J=1,NCOORD
      NEXT=8H
      XIR = PENSEP + XM(J)
      DO 6003 I=1,NOFR
6003 IF(XIR,LE,FRNGX(I)) GO TO 6004
      L=N-NOFR+1
      NEXT=8HEX RIGHT
      GO TO 6011
6004 L=I-1

```



```

      GO TO (6012,6011),I
6012 NEXT=8HEX LEFT
      L=1
6011 FRN01=FRNG+L+(XIR-FRNGX(L))/FGSEP(L+1)
      IF(.NOT.NCAL) GO TO 9000
      FREQ1=A+B*FRN01
      PRINT 9651, NEXT,FRN01,WT(J),FREQ1
      IF(.NOT. IPUNCH) GO TO 6001
      IF(NEXT.NE. 8H          ) GO TO 6001
300  CONTINUE
      IF(.NOT. IOP(2)) GO TO 6001
      IF (ILT,EQ. 1) GO TO 1009
5    IF (FRQ(NAVF,ILT-1) .LE. FREQ1 ) GO TO 6
      FRQ(NAVF,ILT)=FRQ(NAVF,ILT-1)
      WTS(NAVF,ILT)=WTS(NAVF,ILT-1)
      ILT = ILT - 1
      IF (ILT,EQ. 1) GO TO 6
      GO TO 5
6    FRQ(NAVF,ILT)=FREQ1
      WTS(NAVF,ILT)=WT(J)
      GO TO 10
1009 FRQ(NAVF,ILT)=FREQ1
      WTS(NAVF,ILT)=WT(J)
10  IL = IL + 1
12  ILT = IL
      GO TO 6001
8001 IF(.NOT.IOP(3)) GO TO 330
8000 NM=IL-1
      PUNCH 301,(FRQ(NAVF,JJ),WTS(NAVF,JJ),JJ=MD,MM)
      MD=IL
      IF(ICODE.GT.4) 333,71
333  ICARDS=(IL+6)/8
      ILL=IL-1
      PRINT 331,ILL,ICARDS & PUNCH 331,ILL,ICARDS
331  FORMAT (16*FREQUENCIES HAVE BEEN PUNCHED ON*15* CARDS FOR THIS CAS
1E*)
330  CONTINUE
      ILS(NAVF)=ILT
      NAVF=NAVF+1
      GO TO (4,102),ICODE-7
9000 PRINT 9651, NEXT,FRN01,WT(J)
6001 CONTINUE
      GO TO 101
7000 READ3,NHEAD$PRINT3,NHEAD$GOTO101
3    FORMAT (10A8)
100  FORMAT (6(2F5,R1),I1,A4)
106  FORMAT (*0THIS CARD HAS A BLANK OR ZERO CODE* 5X6(2F5,X) /)
301  FORMAT (8(4PF8,R1,X))
6208 FORMAT (**80X*FRINGE SPACING VARIATION ,GT, 10X*)
6209 FORMAT ( 81X*ROTATION FIT ,GT, 10 MICRONS*)
6210 FORMAT (**80X*THETA IS ,GT. 0.005 RADIANS*)
9201 FORMAT(*5*/*1*9A8/* LINE POSITIONS FOR FRAME*      A4,4X*MEASURED BY
1  *2A8)
9300 FORMAT (*6PEN SEPARATION ON THE FILM ==F6.1* MICRONS*)

```



```

9400 FORMAT(*6THE FOLLOWING CALIBRATION CONSTANTS HAVE BEEN INPUT      A
1  =*F11,5*      R =*F13,10)
9500 FORMAT (* FIRST FRINGE IS NO.*F5,8X *ROTATION ANGLE IS*F10,6* RADI
1ANS*/ * ROTATION FITS TO*6(F3*,*)* MICRONS*/ *0FRINGE SEPARATIONS IN
1 MICRONS*/(5X10F5))
9650 FORMAT(*CALIBRATION CONSTANTS USED ARE*5X*A =*F11,5,5X*B =*F13,10)
9651 FORMAT (*9*A9,F10,4,X,R1,F13,4)
9655 FORMAT (/10X*FRINGE NUMBER    FREQUENCY*)
9701 FORMAT (*5*/ *1*9A8)
302  FORMAT(/2A8,18*CARDS*)
      END

```

```

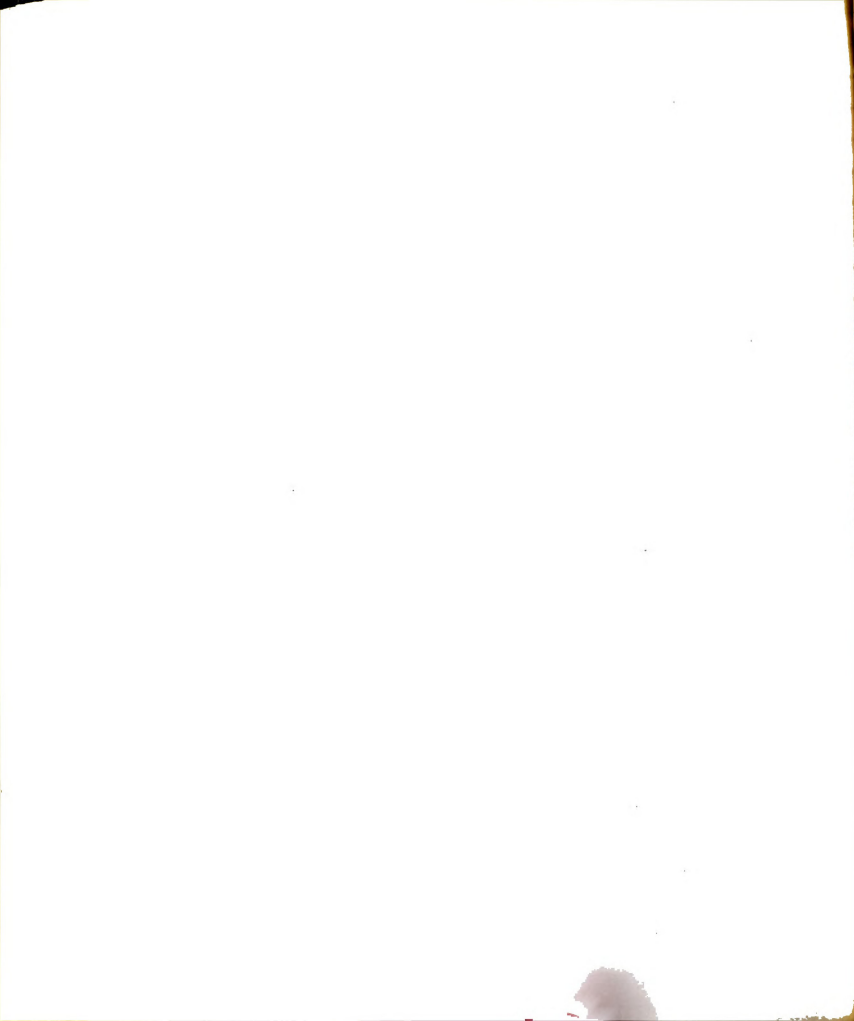
FILE,69
OVERLAY,3,3
FILE END
FTN,L,X

```

```

      PROGRAM AVFRQ(FRQ,WTS,NGPS,IDEM)
      COMMON/1/IOP(3),ILS(8),TOL1,TOL2,TOL3,A,B,LP,IDNT,ICAL,IDON,JUMP
      COMMON/3/NAME1(2000),NAME2(2000),NU(2000),NMAX
      COMMON/5/AVGFRQ(200),AWGT(200),NUM
      COMMON/7/ LL
      COMMON/8/ICHEAD(9),IHEAD(9,2),IDN(4)
      COMMON/9/ CCNT(8,5)
      DIMENSION FRQ(NGPS,IDEM),WTS(NGPS,IDEM)
      DIMENSION FROT(10),I(8),SIG(8),SWT(8),WIT(8),DEV(8),WTT(8),F(10)
      EQUIVALENCE (F,FRQT)
      TYPE INTEGER WTT,WTS,WGT,WIT
      TOL=0.1*TOL1
      IF(TOL.LT.0.0002) TOL=0.0002
      NPUNCH=1
      LL=1
      AZERO=A
      AONE=B
      AVLAST=0.
      NOS=0
      N=NGPS+1
      IF(JUMP) GO TO 2013
      PRINT 260
260  FORMAT(1H9/1H1)
      IF(IDNT) GO TO 1307
1    READ 160,ICHEAD,IFDONE
160  FORMAT(10A8)
      IF(IFDONE .EQ. 8HIDN HEAD) GO TO 1107
      PRINT 160,ICHEAD
      IF(IFDONE .NE. 8HEND HEAD) GO TO 1
      N = 1
      NUM=0
1001 READ 161,(IHEAD(N,J),J=1,2),A,B,IWT
      IF(N .EQ. 1) GO TO 1002
      IF(IHEAD(N,2) .EQ. 8H DELETE) GO TO 50
      IF(IHEAD(N,2) .EQ. 8H CHANGE) GO TO 53
      IF(IHEAD(N,2),FQ.8H PUNCH) 107,108
107  ILTM=ILS(NM1)

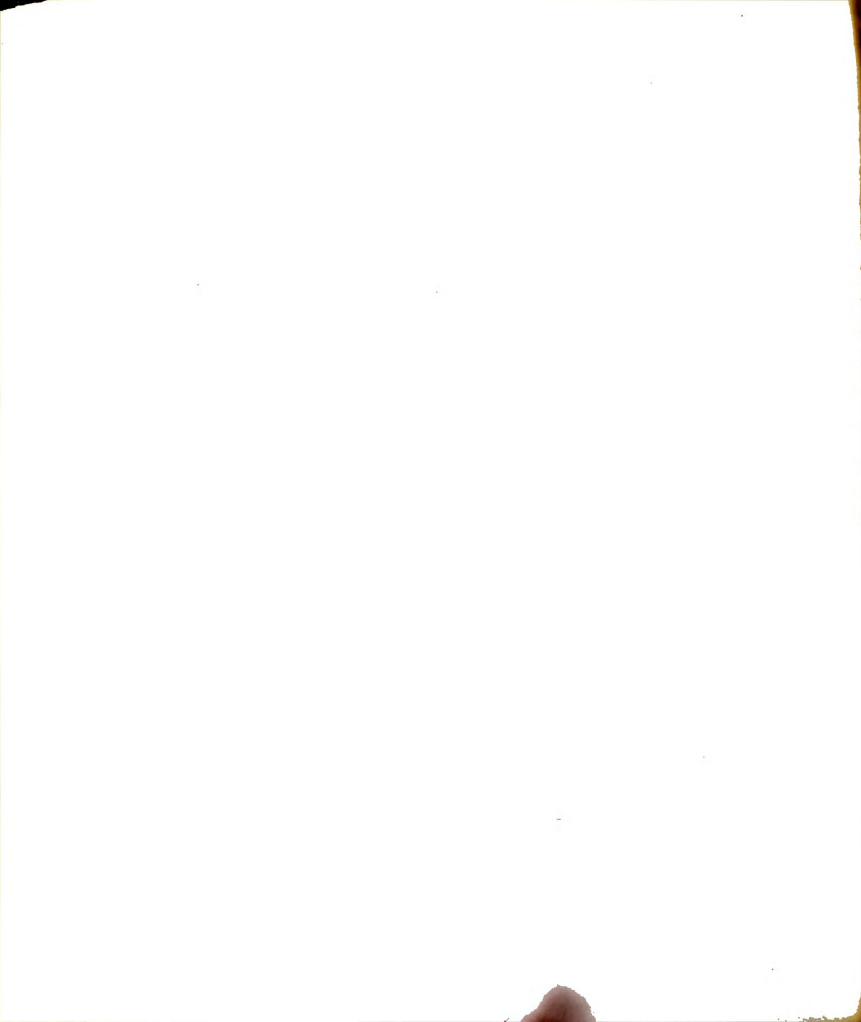
```



```

PUNCH 106, (FRQ(NM1,J),WTS(NM1,J),J=1,ILFM)
GO TO 1001
1107 DO 1207 J=1,4
1207 IDN(J)=ICHEAD(J)
GO TO 1
1307 IDN(3)=8H IDENTIF $IDN(4)=8HICATION $ GO TO 1
108 CONTINUE
IF (N.GT. NGPS) GO TO 13
1002 CONTINUE
CCWT(N,1)=.016 $ CCWT(N,2)=.062 $ CCWT(N,3)=.25 $ CCWT(N,4)=1.0
CCWT(N,5)=1.0
IPRINT=55
IF(A) 71,72
71 IA=A $ IXA=(A-IA)*1.E5 $ IB=B*1.E5 $ XB=B*1.E5 $ IXB=(XB-IB)*1.E5
PUNCH 70, IA,IXA,IB,IXB
70 FORMAT(15X,14,X,15,9X,15,X,15)
72 IL=ILT=ILS(N)
SIG(N)=0.
DEV(N)=0.0
SWT(N)=0.
IF(ICAL.NE.0) GO TO 2
PRINT 261, ICHEAD,(IHEAD(N,J),J=1,2)
2 READ 105, (FRQT(J),WTT(J),J=1,8)
105 FORMAT(8(F8,4,R1,X))
IF(FRQT) 73,82
82 IF(FRQT(2)) 80,81
80 AZERO=1.E5*FRQT(2)+WTT(2)+FRQT(3)*.1
AONE=FRQT(4)+1.E-5*WTT(4)+1.E-6*FRQT(5)
IF(A) 77,78
77 SLOPE = B/AONE
PRINT 79,IL, A,B
GO TO 2
78 PRINT 79,IL, AZERO,AONE
79 FORMAT(*0FREQUENCIES BEGINNING WITH NUMBER*14* WERE CALCULATED USI
1NG*/* THE FOLLOWING CONSTANTS, A=*F11,5* B=*F12,10)
GO TO 2
81 IF(FRQT(3))83,84
83 CCWT(N,1)=FRQT(6)
CCWT(N,2)=FRQT(5)
CCWT(N,3)=FRQT(4)
CCWT(N,4)=FRQT(3)
CCWT(N,5)=FRQT(7)
GO TO 2
73 CONTINUE
IF(A) 74,75
74 DO 76 J=1,8
76 FRQT(J)=A+(FRQT(J)-AZERO)*SLOPE
PUNCH 106,(FRQT(J),WTT(J),J=1,8)
106 FORMAT (8(4PF8,R1,X))
75 DO 12 J=1,8
IF (FRQT(J).EQ. 0) GO TO 12
IF (ILT.EQ. 1) GO TO 1009
5 IF (FRQ(N,ILT-1) .LE. FRQT(J)) GO TO 6
FRQ(N,ILT)=FRQ(N,ILT-1)

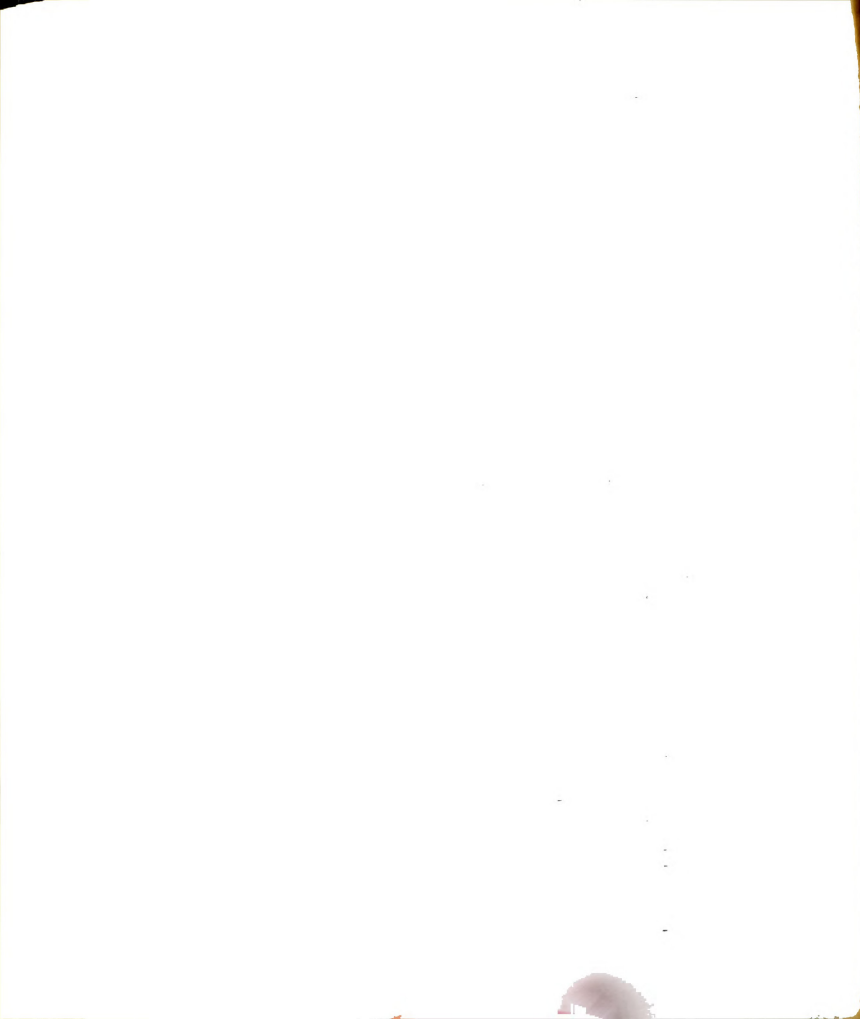
```



```

      WTS(N,ILT)=WTS(N,ILT-1)
      ILT = ILT - 1
      IF (ILT,EQ, 1) GO TO 6
      GO TO 5
6     FRQ(N,ILT)=FRQT(J)
      WTS(N,ILT)=WIT(J)
      GO TO 10
1009  FRQ(N,ILT)=FRQT(J)
      WTS(N,ILT)=WIT(J)
      10 IL = IL + 1
      12 ILT = IL
      IF(FRQT) GO TO 2
      84 CONTINUE
      IF(ICAL .NE. 0) GO TO 3084
      PRINT 2084,(CCWT(N,J),J=1,5)
2084  FORMAT (*0WEIGHT-CODE CORRESPONDENCE*/5X* CODE*6X,*1*9X,*2*9X,*3*
      19X,*4*,7X*BLANK*/* WEIGHT*5F10,4)
3084  CONTINUE
      ILT=ILT-1
      FTOT=FRQ(N,1)
      FRQ(N,IL)=1,E30
      ISAME=1
      IDROP=0
      DO 750 J=1,ILT
      WGT=WTS(N,J)
      IF(FRQ(N,J+1)-FRQ(N,J) ,GT. TOL1) GO TO /10
      FTOT=FRQ(N,J+1)+FTOT
      ISAME=ISAME+1
      IDROP=IDROP+1
      GO TO 750
710   AVF=FTOT/ISAME
      JTT=J-ISAME+1
      IF(IPRINT,LT.50) GO TO 709
      IPRINT=0
      IF(.NOT,A) GO TO 1762
      PRINT 762,ICHEAD,(IHEAD(N,L),L=1,2),A,B,TOL1
      GO TO 709
1762  PRINT 762,ICHEAD,(IHEAD(N,L),L=1,2),AZERO,AONE,TOL1
762   FORMAT(1H1,9A8/1H0,2A8/*0 CALIBRATION CONSTANTS A=*F11,5
      1* R=*F12,10/*0 THESE FREQUENCIES ARE WITHIN*F7,3* WAVE NOS, OF
      2EACH OTHER AVERAGE*/)
709   IF(ISAME-1) 712,711
711   IF(IDON,NE,1) GO TO 720
712   PRINT 760, (FRQ(N,K),WTS(N,K),K=JTT,J)
760   FORMAT(5(F11.4,X,R1))
      IPRINT=IPRINT+(JTT-J+4)/5
      PRINT 761,AVF
761   FORMAT(1H+,67XF10,4)
720   FRQ(N,J-IDROP)=AVF
      WTS(N,J-IDROP)=WGT
      ISAME=1
      FTOT=FRQ(N,J+1)
750   CONTINUE
      ILT=ILT-IDROP

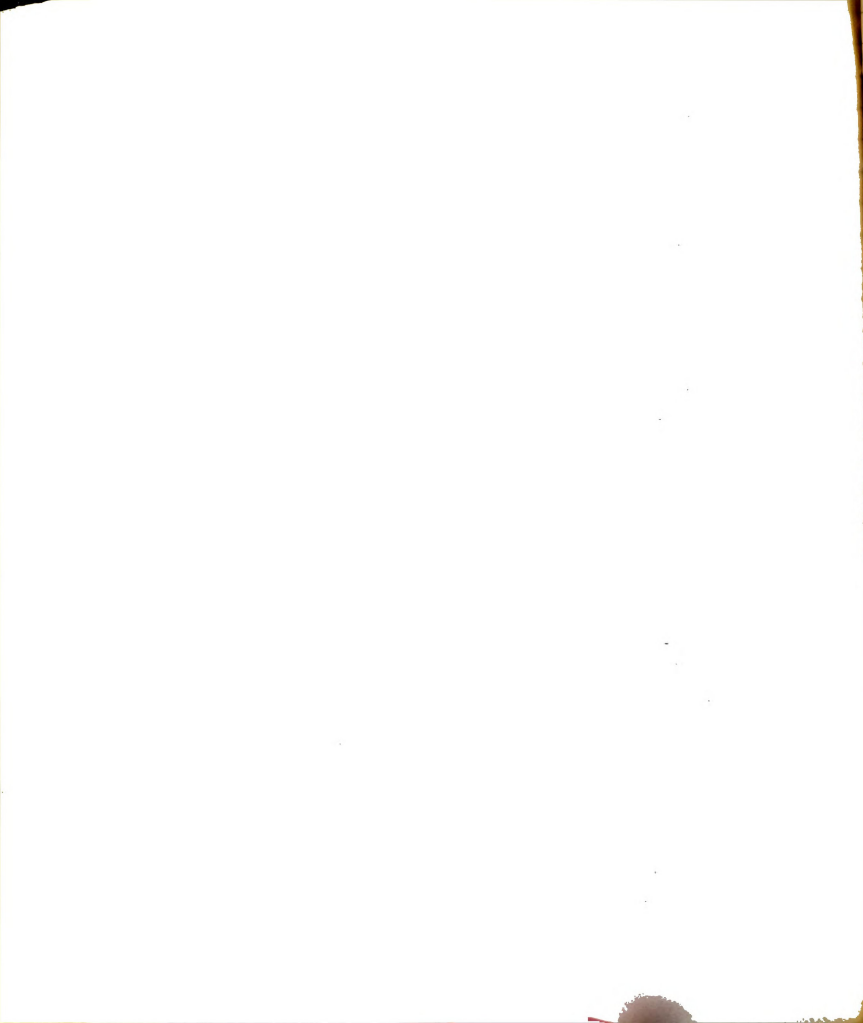
```



```

      ILS (N) = ILT
      IL=ILT+1
      FRQ(N,IL)=1,E20
      NM1=N
      N = N + 1
      GO TO 1001
2013 CONTINUE
      DO 15 NI=1,NGPS
      NILS=ILS(NI)
      DO 15 J=1,NILS
15  FRQ(NI,J)=A+B*FRQ(NI,J)
13  N=N-1
      IF(ICAL .NE. 0) GO TO 1013
      PRINT 261,ICHEAD
      PRINT 269, (IDN(1),IDN (2),(IHEAD(IH,1),IH=1,N))
      PRINT 270,(IDN(3),IDN(4),(IHEAD(IH,2),IH=1,N))
      PRINT 271
      IPRT=0
1013 CONTINUE
      IF(A ,EQ. 0.) A=AZERO
      IF(B ,EQ. 0.) B=AONE
      NM1 = N - 1
      DO 20 J=1,N
20  I(J)=1
32  FS=F(1)=FRQ(1,I(1))
      SIGT=0.
      WIT(1)=WTS(1,I(1))
      DO 34 K=2,N
      F(K)=FRQ(K,I(K))
      IF(F(K) ,LT. FS) FS=F(K)
      WIT(K)=WTS(K,I(K))
34  CONTINUE
      AVG=AVW=0
      ICNT=0
      DO 36 K=1,N
      IF(F(K)*FS ,LE. TOL2) GO TO 35
      F(K)=1.E20
      WJT(K)=48
      GO TO 36
35  XCWT=CWT(K,WIT(K))
      AVG=AVG+F(K)*XCWT
      AVW=AVW+XCWT
      I(K)=I(K)+1
      ICNT=ICNT+1
36  CONTINUE
      AVG=AVG/AVW
      IAVG=AVG
      DO 38 K=1,N
      IF(F(K) ,GT. 1.E10) GO TO 38
      IF(ICNT ,LE. 1) GO TO 37
      XCWT=CWT(K,WIT(K))
      DEVT=(AVG-F(K))
      SIGST=DEVT**2*XCWT
      SIG(K)=SIG(K)+SIGST

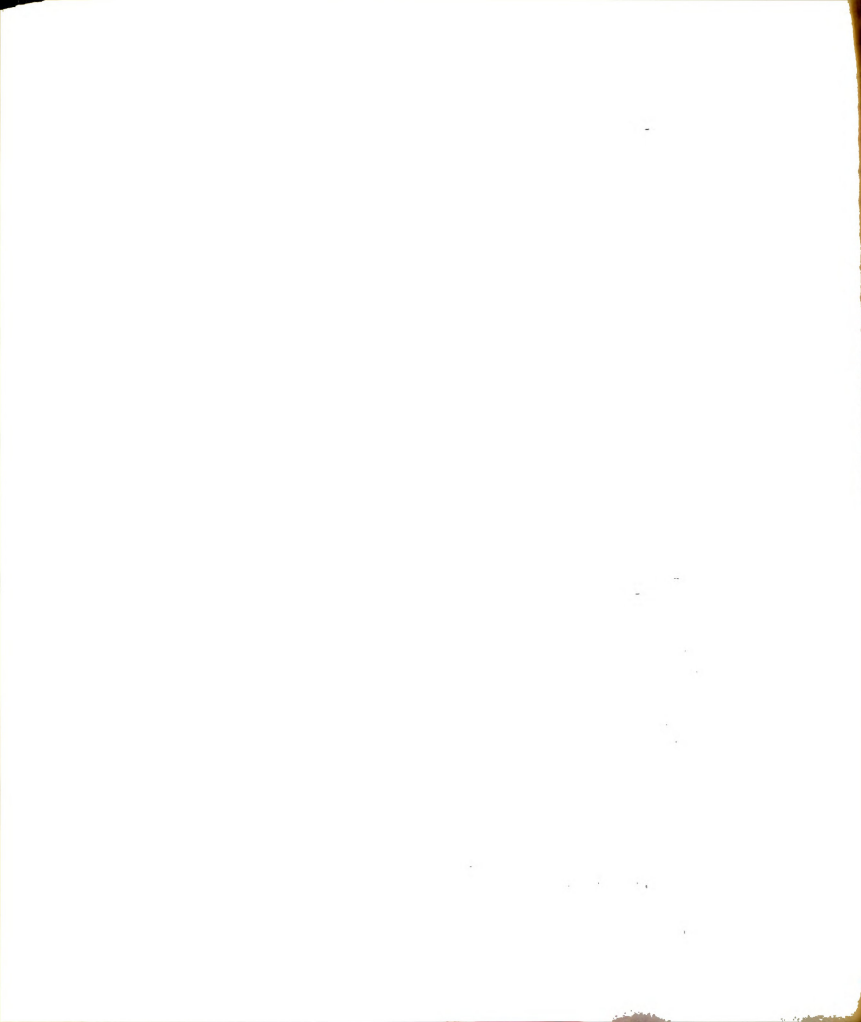
```




```

      SIGT=SIGT+SIGST
      DEV(K)=DEV(K)+DEVT*XCWT
      SWT(K)=SWT(K)+XCWT
37  F(K)=F(K)-IAVG
      IF(F(K) .LT. 0) F(K)=1.+F(K)
38  CONTINUE
      SIGT=SQRT((SIGT*ICNT)/((ICNT-1)*AVW))
      IPRT=IPRT+1
      IF(IPRT .LE. 50) GO TO 370
      PRINT 262,TOL2
      PRINT 261,ICHEAD
      PRINT 269, (IDN(1),IDN(2),(IHEAD(IH,1),IH=1,N))
      PRINT 270,(IDN(3),IDN(4),(IHEAD(IH,2),IH=1,N))
      PRINT 271
      IPRT=1
370  CONTINUE
      FRNG=(AVG-A)/B
      IF(IDNT) 8250,8300
8250  CALL IIDENT(AVG)
8300  IF(ICAL) 2000,2001
2000  NUM=NUM+1
      AVGFREQ(NUM)=AVG $ AWGT(NUM)=AVW
      GO TO 1270
2001  PRINT210,NAME1(LP),NAME2(LP),FRNG,AVG,AVW,SIGT,(F(J),WIT(J),J=1,N)
      IF(IDP(2).NE.2) GO TO 570
      IF(IDON,EQ.2) 1280,1290
1280  PUNCH 1210, NAME1(LP),NAME2(LP),AVG
      GO TO 570
1290  IF(NAME1(LP) .EQ. 8H          ) GO TO 570
      PUNCH 1210, NAME1(LP),NAME2(LP),AVG,AVW
570  CONTINUE
      IF(AVG-AVLAST .GT. TOL2) GO TO 1270
      IF(ABS(AVG-AVLAST) .GT. TOL2) GO TO 1270
      PRINT 276
1270  CONTINUE
      AVLAST=AVG
27  DO 28 J = 1,N
      IF (I(J) .LE. ILS(J)) GO TO 32
28  CONTINUE
      IF(ICAL .NE. 0) GO TO 60
      GSIGT=0.
      GAVW=0.
      NUMB=0
      DO 56 J = 1,N
      NUMB=NUMB+ILS(J)
      DEV(J)=DEV(J)/SWT(J)
      GSIGT=GSIGT+SIG(J)
      GAVW=GAVW+SWT(J)
56  SIG(J)=SQRT(SIG(J)*ILS(J)/(ILS(J)-1)/SWT(J))
      GSIGT=SQRT(GSIGT*NUMB/(NUMB-1)/GAVW)
      PRINT 235,(DEV(J),J=1,N)
235  FORMAT(*0 AVERAGE DEVIATION*30X,8(3XF7,4))
      PRINT 230,GSIGT,(SIG(J) ,J=1,N)
230  FORMAT (* STANDARD DEVIATION*24XF7,4,2XF7.4,7(3XF7,4))

```



```

      PRINT 240,(ILS(J),J=1,N)
240  FORMAT (* NO. OF LINES MEASURED*26X,8(6X14))
      PRINT 262,TOL2
      GO TO 60
50   CONTINUE
      DO 52 K=1,ILT
      IF(ABS(FRQ(NM1,K)-A) .GT. TOL) GO TO 52
      DO 51 J=K,ILT
      WTS(NM1,J)=WTS(NM1,J+1)
51   FRQ(NM1,J)=FRQ(NM1,J+1)
      ILS(NM1)=ILS(NM1)-1
      ILT=ILS(NM1)
      GO TO 1001
52   CONTINUE
      PRINT 280,A,IHEAD(N,2)
      GO TO 1001
53   CONTINUE
      DO 54 K=1,ILT
      IF(ABS(FRQ(NM1,K)-A) .GT. TOL) GO TO 54
      IF(B .LT. FRQ(NM1,K)) GO TO 1053
      DO 1054 KQK=K,ILT
      IF(B .GT. FRQ(NM1,KQK+1)) GO TO 1054
      WTS(NM1,KQK)=IWT
      FRQ(NM1,KQK)=B
      GO TO 1001
1054 FRQ(NM1,KQK)=FRQ(NM1,KQK+1)
      WTS(NM1,KQK)=WTS(NM1,KQK+1)
      FRQ(NM1,ILT)=B
      WTS(NM1,ILT)=IWT
      GO TO 1001
1053 KM1=K-1
      DO 1055 KQK=1,KM1
      KQM=K-KQK
      IF(B .LT. FRQ(NM1,KQM)) GO TO 1055
      FRQ(NM1,KQM+1)=B
      WTS(NM1,KQM+1)=IWT
      GO TO 1001
1055 FRQ(NM1,KQM+1)=FRQ(NM1,KQM)
      WTS(NM1,KQM+1)=WTS(NM1,KQM)
      FRQ(NM1,1)=B
      WTS(NM1,1)=IWT
      GO TO 1001
54   CONTINUE
      PRINT 280,A,IHEAD(N,2)
      GO TO 1001
60   CONTINUE
9500 RETURN
161  FORMAT (2A8,4X,2E15,10,X,R1)
210  FORMAT (1X,2A8,F8.2,F11.4,F6.2,XF7.4,X8(2XF6.4,X,R1))
261  FORMAT(1H1,10A8/1H02A8/1H0)
262  FORMAT (*NOTE.. LINES ARE ASSUMED TO BE THE SAME IF FREQUENCIES*
1*      ARE WITHIN*F7,3* WAVE NOS. OF EACH OTHER,*/*5*)
269  FORMAT (*0*2A8,2X*FRINGE   AVERAGE*10X*STD.*2X8A10)
270  FORMAT (1X2A8,2X*NUMBER   FREQUENCY   WGT,   DEV.*2X8A10)

```



```

271  FORMAT (1H )
272  FORMAT (** IDENTIFICATION*)
276  FORMAT (**+35X,1H*)
280  FORMAT(*FREQUENCY OF*F10,4* WAS NOT PRESENT TO*A8)
1210 FORMAT(2A8,3X,F13,4,7X,F4,2)
9650 FORMAI (10I8)
      FND

```

```

      FUNCTION CWT(IA,IB)
      COMMON/9/ CCWT(8,5)
      IF(IB,EQ.0) GO TO 3
      IF(IR,GT.4) GO TO 4
      CWT=CCWT(IA,IB)
      RETURN
3    CWT=1,E=20
      RETURN
4    CWT=CCWT(IA,5)
      RETURN
      END

```

```

      SUBROUTINE IIDFNT(AVFREQ)
      COMMON/1/IOP(3),ILS(8),TOL1,TOL2,TOL3,A,B,LP,IDNT,ICAL,IDON,JUMP
      COMMON/3/NAME1(2000),NAME2(2000),NU(2000),NMAX
      COMMON/7/ LL
      TYPE REAL NU
      LP=NMAX+1
40   X=AVFREQ-NU(LL)
      IF(ABS(X),LE,TOL3) 50,60
60   IF(X) 70,70,90
70   RETURN
90   LL=LL+1
      IF(LL,GT,NMAX) IDNT=0
      GO TO 40
50   LP=LL
      IF(ABS(AVFREQ-NU(LL+1)),LE,TOL3) LP=NMAX+2
      RETURN
      END

```

```

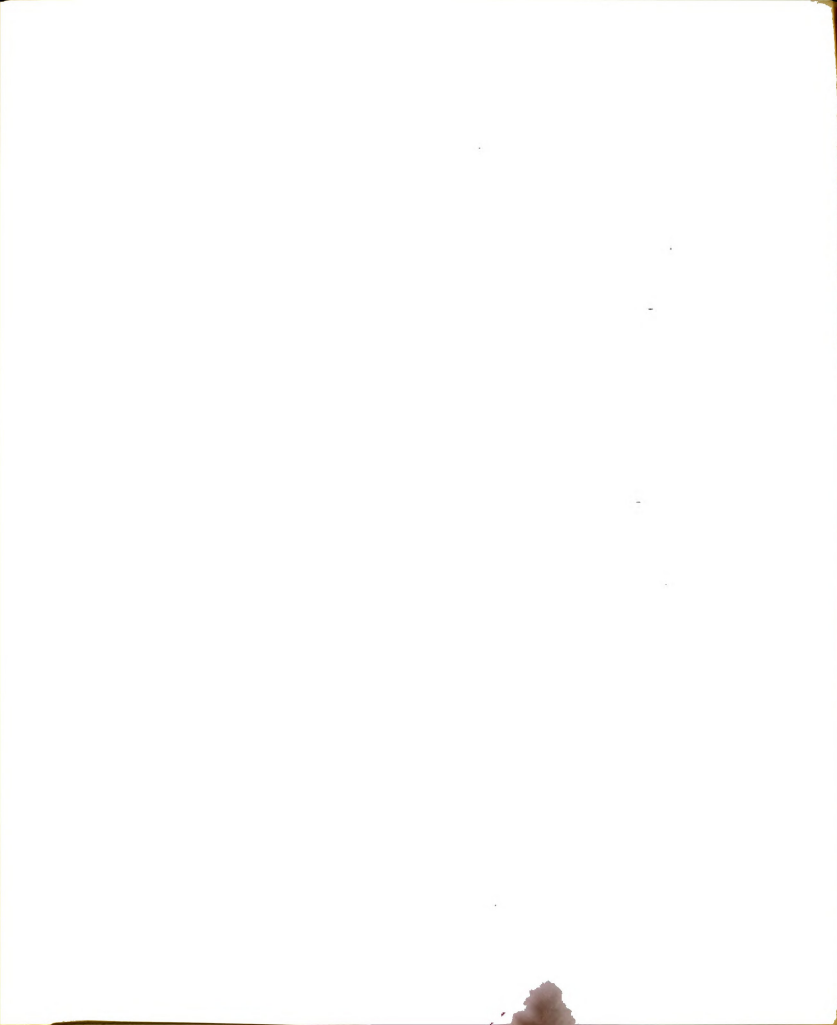
FILE,69
OVERLAY,4,4
FILE END
FTN,L,X

```

```

      PROGRAM SEARCH
      COMMON/1/IOP(3),ILS(8),TOL1,TOL2,TOL3,A,B,LP,IDNT,ICAL,IDON,JUMP
      COMMON/3/NAME1(2000),NAME2(2000),NU(2000),NMAX
      COMMON/4/ FNUM(200),FREQ(200),WT(200),SUMWHT,NODATA,INDATA
      COMMON/5/AVGFREQ(200),AWGT(200),NUM
      DIMENSION IDENT1(200),IDENT2(200)
      TYPE REAL NU
      READ 2, NUMLINES
      SUMWHT=NODATA=INDATA=0.0
      L=1
      LT=1

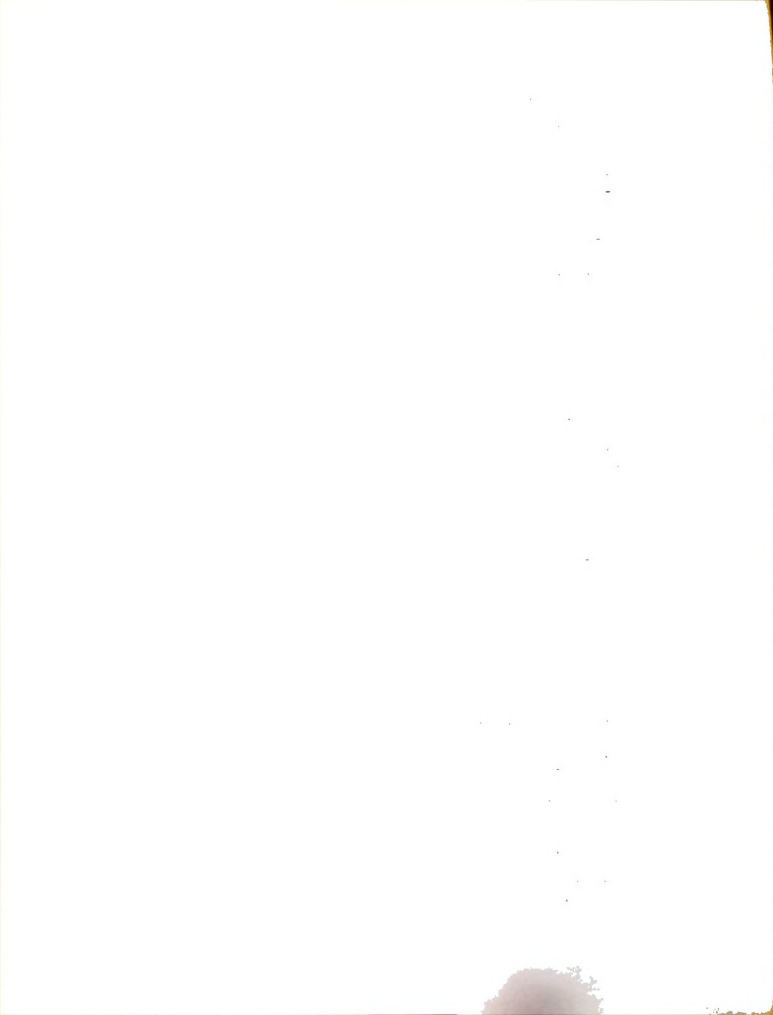
```



```

30 READ 1,IDENT1,IDENT2,XFNUM
   IF(XFNUM,EQ,0,0) GO TO 27
   IF(L,EQ,1) GO TO 6
5  IF(XFNUM(LT-1),LE,XFNUM) GO TO 6
   FNUM(LT)=XFNUM(LT-1)
   IDENT1(LT)=IDENT1(LT-1) $ IDENT2(LT)=IDENT2(LT-1)
   LT=LT-1
   IF(LT=1) 6,0,5
6  FNUM(LT)=XFNUM $ IDENT1(LT)=IDENT1 $ IDENT2(LT)=IDENT2
   L=L+1 $ LT=L $ GO TO 30
27 LMAX=L-1
   IL=LMAX
   IF(LMAX,LT,2) GO TO 1000
   SUMX=SUMY=SUMXY=SUMX2=0,0
   II=0
   IL=1
   DO 50 L=1,LMAX
   DO 49 N=1,NMAX
   IF(IDENT1(L),EQ,NAME1(N)) 31,49
31 IF(IDENT2(L),EQ,NAME2(N)) 32,49
32 X=FNUM(L)-AVGFREQ(LL)
   IF(ABS(X),LE,1,0) 33,34
34 IF(X) 49,49,91
91 LL=LL+1 $ IF(LL,GT,NUM) GO TO 52 $ GO TO 32
33 FNUM(L)=AVGFREQ(LL)
   WT(L)=AWGT(LL)
   FREQ(L)=NU(N)
   SUMWHT=SUMWHT+WT(L)
   IF(WT(L)) 300,301
300 NODATA=NODATA+1
301 NUM=NUM+1 $ II=II+1
40 DO 41 K=LL,NUM
   AVGFREQ(K)=AVGFREQ(K+1)
41 AWGT(K)=AWGT(K+1)
   SUMX=SUMX+FNUM(L)
   SUMY=SUMY+FREQ(L)
   SUMXY=SUMXY+FNUM(L)*FREQ(L)
   SUMX2=SUMX2+FNUM(L)*FNUM(L)
   GO TO 50
49 CONTINUE
   IL=IL+1 $ IF(IL,LT,2) GO TO 1000
50 CONTINUE
52 IF(II,LT,2) GO TO 1000
   D=(II*SUMX2-SUMX*SUMX
   A=(SUMY+SUMX2-SUMX*SUMXY)/D
   B=(II*SUMXY-SUMX*SUMY)/D
   LL=1
   DO 200 IT=1,2
   DO 100 I=1,NUM
   FRO=A+R*AVGFREQ(I)
60 X=FRO-NU(LL)
   IF(ABS(X),LE,TOL3) 76,62
62 IF(X) 100,100,64
64 LL=LL+1 $ IF(LL,GT,NMAX) GO TO 101 $ GO TO 60

```

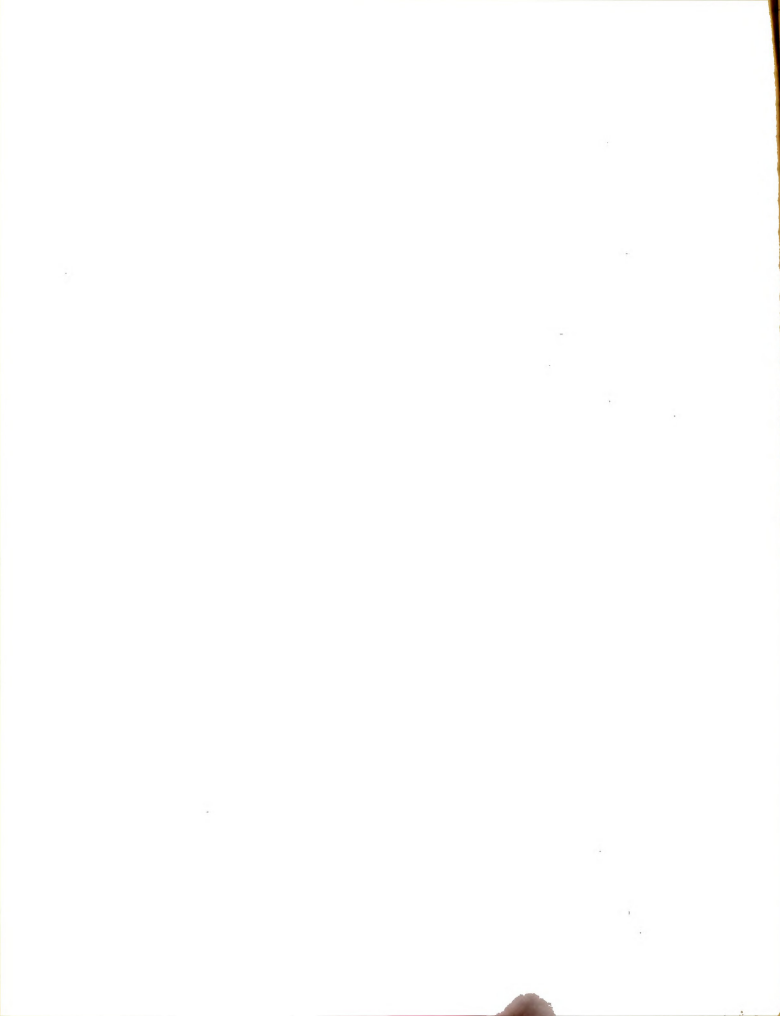



```

76  I1=I1+1
    FRFQ(I1)=NU(LL)
    FNUM(I1)=AVGFREQ(I)
    WT(I1)=AWGT(I)
    SUMWHT=SUMWHT+WT(I1)
    IF(WT(I1)) 400,401
400  NODATA=NODATA+1
401  NUM=NUM+1
    DO 51 K=I,NUM
    AVGFREQ(K)=AVGFREQ(K+1)
51  AWGT(K)=AWGT(K+1)
    I=I-1
80  SUMX=SUMX+FNUM(I1)
    SUMY=SUMY+FREQ(I1)
    SUMXY=SUMXY+FNUM(I1)*FREQ(I1)
    SUMX2=SUMX2+FNUM(I1)*FNUM(I1)
    D=I1*SUMX2-SUMX*SUMX
    A=(SUMY*SUMX2-SUMX*SUMXY)/D
    B=(I1*SUMXY-SUMX*SUMY)/D
100  CONTINUE
101  IF(I1.LT.NUMLINES) 200,201
200  CONTINUE
201  INDATA=I1
    CALL CALFIT
    PRINT 500,INDATA,NUMLINES
    DO 550 K=1,INDATA
550  PUNCH 600,FREQ(K),FNUM(K),WT(K)
    RETURN
1000 PRINT 1001
    RETURN
1  FORMAT(2A8,13X,F10,33X,A8)
2  FORMAT (I10)
500  FORMAT (*2 *15* LINES OUT OF *15* HAVE BEEN FOUND AND ENTERED*)
600  FORMAT (2F15.4,F15.2)
1001 FORMAT(*2A WRONG IDENTIFICATION OR FRINGE NUMBER HAS BEEN INPUT*)
    END

SURROUTINE CALFIT
COMMON/1/IOP(3),ILS(8),TOL1,TOL2,TOL3,A,B,LP,IDNT,ICAL,IDON,JUMP
COMMON/4/ FRINGE(200),FREQ(200),WHT(200),SUMWHT,NODATA,INDATA
DIMENSION COEN(3),DATA(3),IH(10),INDEX(3),SIGMA(3),SIGMCO(3),
1VECTOR(4,4),IHEAD(2)
DATA (IHEAD=8H CONST,8H SLOPE)
TYPE DOUBLE COEN,SIGMA,SIGY,VECTOR
PRINT 3
3  FORMAT(*1*)
99  READ2,IH$IF(IH(10),EQ,8HLAST FIT)STOP$IF(IH(10)-8HEND HEAD)110,115
110 PRINT 2,IH$GO TO 99
115 PRINT2,(IH(I),I=1,9)$NDEL=0
495 DEVMAX=FLEVEL=VAR=0,0$NOIN=K=NOENT=NOMIN=NOMAX=0
501 AVGWHT=SUMWHT/NODATA
    DO 120 I=1,16
120 VECTOR(I )=0,0$DATA=1,0
    DO220N=1,INDATA

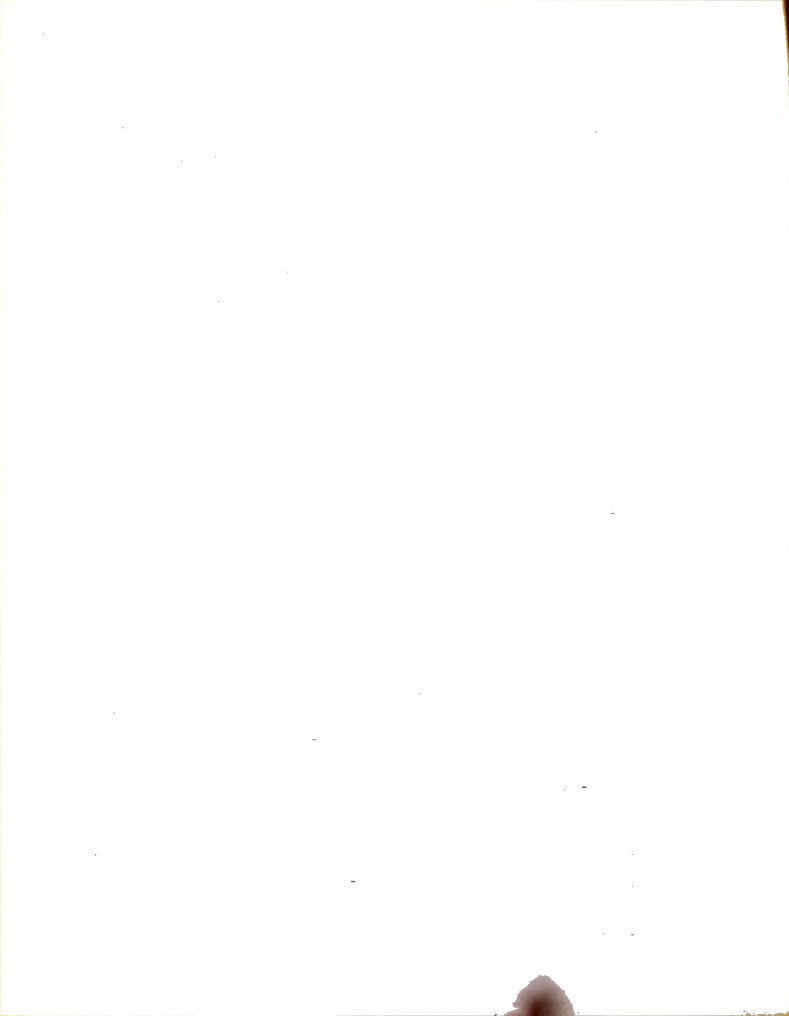
```



```

      WT=WHT(N)/AVGWHT$DATA(2)=FRINGE(N)$DATA(3)=FREQ(N)
      DO220 I=1,3$VECTOR(1,4)=VECTOR(1,4)+DATA(1)*WT$DO220 J=1,3
220  VECTOR(1,J)=VECTOR(1,J)+DATA(1)*DATA(J)*WT
      VECTOR(4,4)=NODATA          $PRINT90,NODATA,AVGWHT,VECTOR(2,4),
1  VECTOR(3,4),VECTOR(2,2),VECTOR(2,3),VECTOR(3,3)$NOSTEP=-1
      DEFR=VECTOR(4,4)-1.0$DO800 I=1,3$IF(VECTOR(1,I)) 792,794,810
792  PRINT793,1$GOTO100
794  PRINT795,1$SIGMA(I)=1.0$GOTO800
810  SIGMA(I)=DSQRT(VECTOR(1,I))
800  VECTOR(1,I)=1.0$DO830 I=1,2$IP1=I+1$DO830 J=IP1,3
830  VECTOR(J,I)=VECTOR(1,J)=VECTOR(1,J)/SIGMA(I)/SIGMA(J)
      PRINT60,VECTOR(2,1),VECTOR(3,1),VECTOR(3,2)
1000  NOSTEP=NOSTEP+1$IF(VECTOR(3,3))1002,1002,1010
1002  NSTPM1=NOSTEP-1$PRINT1004,NSTPM1$GOTO1381
1010  SIGY=SIGMA(3)*DSQRT(VECTOR(3,3)/DEFR)$DEFR=DEFR-1.0
      IF(DEFR) 1017,1017,1020
1017  PRINT1019,NOSTEP$GOTO1381
1020  VMIN=VMAX=0.0$NOIN=0$DO1050 I=1,2$IF(VECTOR(1,I)) 1042,1050,1060
1042  PRINT1044,1,NOSTEP$GOTO1381
1060  IF(VECTOR(1,I)-0.0001) 1050,1080,1080
1080  VAR=VECTOR(1,3)*VECTOR(3,I)/VECTOR(1,I)$IF(VAR)1100,1050,1110
1100  NOIN=NOIN+1$INDEX(NOIN)=I$COEN(NOIN)=VECTOR(1,3)*SIGMA(3)/SIGMA(I)
      SIGMCO(NOIN)=DSQRT(VECTOR(1,I))*SIGY/SIGMA(I)
      IF(VMIN) 1160,1170,904
904  PRINT906$GOTO100
1170  VMIN=VAR$NOMIN=I$GOTO1050
1160  IF(VAR-VMIN)1050,1050,1170
1110  IF(VAR-VMAX)1050,1050,1210
1210  VMAX=VAR$NOMAX=I
1050  CONTINUE$IF(NOIN)903,1240,1310
903  PRINT907$GOTO100
1240  PRINT65,SIGY$GOTO1350
1310  IX=8$ENTERING$IF(NOENT)1311,1311,1313
1311  IX=8$REMOVED
1313  PRINT91,NOSTEP,IX,IHEAD(K)
1314  PRINT 70,IHEAD(K),FLEVEL,SIGY
      DO 71 J=1,NOIN
      JK=INDEX(J)
71  PRINT 72,IHEAD(JK),COEN(J),SIGMCO(J)
      A=COEN(1)  B=COEN(2)
72  FORMAT (A17,F18.10,F16.10)
1320  FLEVEL=VMIN*DEFR/VECTOR(3,3)$IF(FLEVEL+0.0000001)1350,1350,1340
1340  K=NOMIN$NOENT=0$GOTO1391
1350  FLEVEL=VMAX*DEFR/(VECTOR(3,3)-VMAX)
      IF(FLEVEL+0.0000001) 1380,1370,1370
1370  NOENT=K=NOMAX
1391  IF(K)1392,1392,1400
1392  PRINT1395,NOSTEP$GOTO100
1400  VK=1.0/VECTOR(K,K)$DO1410 I=1,3$IF(I-K)1430,1410
1430  DO1440 J=1,3
1440  IF(J,NE,K) VECTOR(I,J)=VECTOR(I,J)+VECTOR(I,K)*VECTOR(K,J)*VK
1410  CONTINUE
      DO 1480 I=1,3
1480  IF(I,NE,K) VECTOR(I,K)=-VECTOR(I,K)*VK

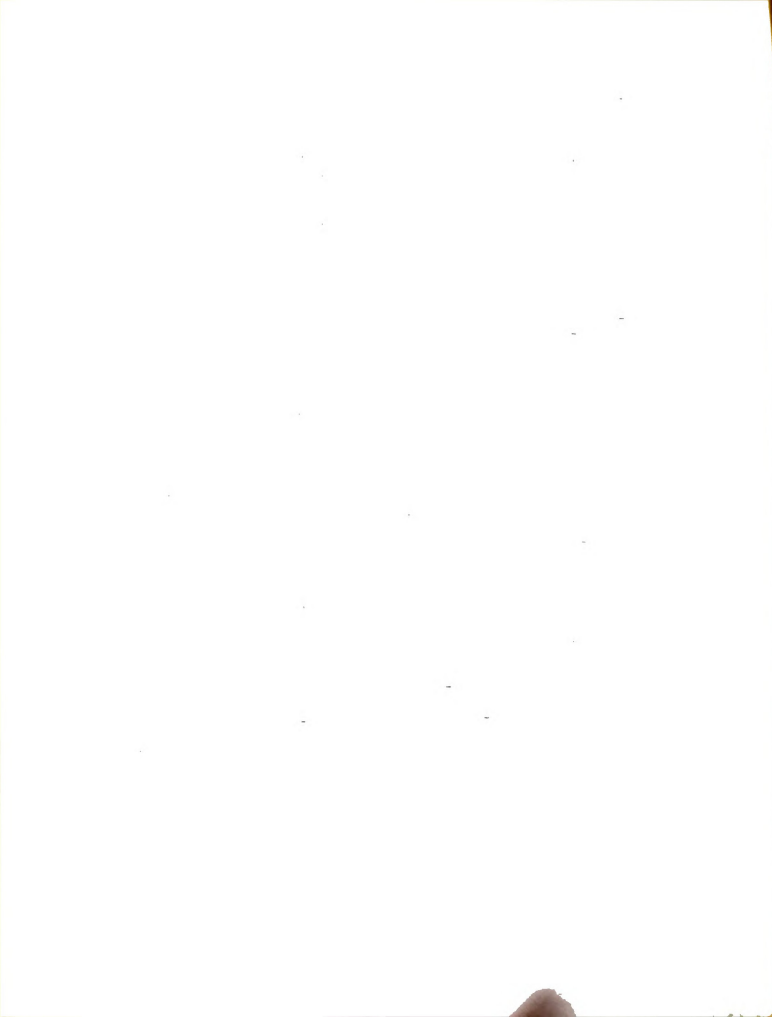
```



```

DO 1520 J=1,3
1520 IF(J,NE,K) VECTOR(K,J)=VECTOR(K,J)*VK
    VECTOR(K,K)=VK$GOTO1000
1380 PRINT 75,NOSTEP
1381 CONTINUE
1580 PRINT1586,VECTOR(1,1),VECTOR(2,2)$VFIT=0,$DATA=1,$DO1660N=1,INDATA
    WT=WHT(N)$DATA(2)=FRINGE(N)$YPRED=0,0$DO1630I=1,N0IN
1630 YPRED=YPRED+COEN(I)*DATA(1)$DEV=FREQ(N)-YPRED
    VFIT=VFIT+WT*DEV*DEV$PRINT9050,N,DATA(2),FREQ(N),YPRED,DEV,WT
    ADEV=WT*DEV*DEV$IF(ADEV-DEVMAX)1660,1610,1610
1610 NMAX=N
    DEVMAX=ADEV
1660 CONTINUE
    VFIT=VFIT*NODATA/(NODATA-2.0)/VECTOR(4,4)
    STDFIT=DSQRT(VFIT)$PRINT1,VFIT,STDFIT
    IF(5-NDEL)100,100,1624
1624 IF(DEVMAX=0,000025)100,100,1620
1620 NDEL=NDEL+1$NODATA=NODATA-1$SUMWHT=SUMWHT-WHT(NMAX)$WHT(NMAX)=0.0
    PRINT 9001,NMAX
    GO TO 495
100 RETURN
1 FORMAT (*0VARIANCE =*F11.6/* STD. DEV. =*F8.4/*7*)
2 FORMAT (10A8)
60 FORMAT (*0PARTIAL CORRELATION COEFFICIENTS*9X*CONST FRINGE*/28X*
1FRINGE*F12.4/28X*FREQUENCY*2F9.4)
65 FORMAT (*0STANDARD ERROR OF Y IS*F12.6)
70 FORMAT(* F LEVEL OF*R6,E11.2/* STD DEV OF (O-P)*E11.2//10X*VARIABLE
1F COEFFICIENT STD. ERROR*/)
75 FORMAT (*0COMPLETED*I2* STEPS OF REGRESSION*)
90 FORMAT(*-CALIBRATION FIT OF*I4* LINES*/*0WEIGHT NORMALIZATION*F5.2
1/* SUM OF FRINGE NOS, IS*F12.4/* SUM OF FREQUENCIES IS*F12.4/*0DRAW
1 SSCP MATRIX FRINGE FREQUENCY/* FRINGE*F18.2/* FR
2FREQUENCY*2F15.2)
91 FORMAT (*0STEP NO,*I2* VARIABLE*A9,A8)
793 FORMAT (*ERROR RESID. SQUARE VAR,*I2* IS NEGATIVE. SO LONG*)
795 FORMAT (*0VARIABLE*I2* IS CONSTANT*)
906 FORMAT (*0ERROR, VMIN PLUS, SO LONG*)
907 FORMAT (*0ERROR, NOIN MINUS, SO LONG*)
1004 FORMAT (*0Y SQUARE NON-POSITIVE, TERMINATE STEP*I2)
1019 FORMAT (*0NO MORE DEGREES FREEDOM STEP*I2)
1044 FORMAT (*0SQUARE X=*I1* NEGATIVE, SO LONG*I2* STEPS*)
1395 FORMAT (*0K=0 STEP*I2*, SO LONG*)
1586 FORMAT(*0DIAGONAL ELEMENTS*5X*CONST*F9.4/23X*FRINGE*F8.4/*1*10X*RE
1SULTS*/*0 RUN FRINGE FREQ OBS FREQ CALC OBS-CALC WHT*/)
9000 FORMAT (3F15,27XA8)
9001 FORMAT (*+DELETING LINE NO,*I4)
9050 FORMAT (I4,F10.4,2F11.4,F9.4,F6,2)
END

```



B. DIFF

This program reads and stores punch output from SHAFT and obtains the Λ -doublet splittings, and the weighted average of all possible rotational combination differences, vibrational differences and spin-orbit differences. Average Λ -doublet frequencies are calculated and punched.

STRUCTURE OF DATA DECK

I. Frequencies

Up to 600 lines may be input.

<u>Col.</u>	<u>Field</u>	<u>Variable</u>
1	I	Upper vibrational state of line.
9	R	Branch of the line (P, Q, and R).
10	R	Subband (1, 2, H, L).
12-13	I	Lower state J value times 2.
16	R	+/- indicating Λ -doublet component.
20-33	F	Line frequency.
41-44	F	Weight of line.
73-80	A	"END DATA" signals end of data.

II. Options

1. Punch card: PUNCH in cols. 76-80 indicates that punch output of difference is desired for input to fitting programs.
2. Heading cards: Cols. 1-72 are printed until END HEAD is encountered in cols. 73-80. The last card is printed at the top of each page.



3. Any of the following may appear:

- a) RTCOMDIF in cols. 73-80 indicates that rotational combination differences are desired. In the first 8 cols. of this card a tolerance may be read, equal to 0.001 times the integer number appearing. This is used to print a flag if two or more differences are averaged which differ by more than this number.
- b) VIBRADIF in cols. 73-80 indicates that vibrational differences are desired.
- c) SPORDIF1,2 in cols. 73-80 indicate that spin-orbit differences are desired, for the ground and excited vibrational states respectively.
- d) END CALC in cols. 73-80 terminates execution.

(Note: If Λ -doublets are present in the input data, a punch output of the average frequencies is automatically given in the frequency input format.)

A listing of the program follows.

3. Any of the following may appear:

- a) RTCOMDIF in cols. 73-80 indicates that rotational combination differences are desired. In the first 8 cols. of this card a tolerance may be read, equal to 0.001 times the integer number appearing. This is used to print a flag if two or more differences are averaged which differ by more than this number.
- b) VIBRADIF in cols. 73-80 indicates that vibrational differences are desired.
- c) SPORDIF1,2 in cols. 73-80 indicate that spin-orbit differences are desired, for the ground and excited vibrational states respectively.
- d) END CALC in cols. 73-80 terminates execution.

(Note: If Λ -doublets are present in the input data, a punch output of the average frequencies is automatically given in the frequency input format.)

A listing of the program follows.

```

PROGRAM DIFF
COMMON/1/NU(600),WGT(600),JU(600),JL(600),VU(600),SU(600),SL(600),
1 JUMP,N,DSODIFF(100,1),SODIFF(100,3),DWT(100,1),WT(100,3)
COMMON/2/ LAMDA(600),ISUR(600)
COMMON/3/ ICODE(9), IPUN
COMMON/4/ TOL
DIMENSION ICODE(10)
TYPE REAL NU
TYPE INTEGER VU,SU,SL,BRANCH,STP
N=1
NLines=NTOTAL=0
1 READ 2,VU(N),BRANCH,ISUB(N),JLW,LAMDA(N),NU(N),WGT(N),STP
IF(STP.EQ.9999) GO TO 20
JLW=(JLW+1)/2
IF(BRANCH-100) 3,4,5
3 JU(N)=JLW-1
GO TO 6
4 JU(N)=JLW
GO TO 6
5 JU(N)=JLW+1
6 JL(N)=JLW
IF(ISUR(N)-2) 8,9,11
8 SU(N)=SL(N)=1 & GO TO 7
9 SU(N)=SL(N)=2 & GO TO 7
11 IF(ISUR(N).EQ.100) 12,13
12 SL(N)=1 & SU(N)=2 & GO TO 7
13 SL(N)=2 & SU(N)=1
7 N=N+1
GO TO 1
20 N=N-1
DO 10 LL=1,N
IF(LAMDA(LL).NE.100) 15,10
15 CALL LAMDAIF
GO TO 95
10 CONTINUE
GO TO 100
95 PRINT 50
PRINT 51
DO 18 I=1,N
BRANCH=JU(I)+JL(I)+40
JLOWER=2*JL(I)-1
PRINT 300, VU(I),BRANCH,ISUB(I),JLOWER,LAMDA(I),NU(I),WGT(I)
PUNCH 301, VU(I),BRANCH,ISUB(I),JLOWER,LAMDA(I),NU(I),WGT(I)
NLines=NLines+1
NTOTAL=NTOTAL+1
IF(NLines.GE.50) 17,18
17 PRINT 53
PRINT 51
NLines=0
18 CONTINUE
PRINT 54, N
100 JUMP=0
IPUN=0
ASSIGN 75 TO NGO

```

```

70 READ 101, ICODE
   IF(ICODE(10).EQ.8H PUNCH) GO TO 1000
   GO TO NG0
1000 IPUN=1
   GO TO 70
   75 IF(ICODE(10)-8HEAD CALC) 80,110
   80 IF(ICODE(10).EQ.8HEND HEAD) GO TO 200
   90 PRINT 150, (ICODE(I),I=1,9)
   GO TO 70
200 ASSIGN 102 TO NG0
   DO 201 I=1,9
201 NCODE(I)=ICODE(I)
   GO TO 90
102 IF(ICODE(10)-8HRTCOMDIF)104,103
103 TOL=.001*ICODE(1)
   CALL RTCOMDIF
   GO TO 100
104 IF(ICODE(10)-8HSPORDIF1)106,105
105 TOL=.001* ICODE(1)
   CALL SPORDIF1
   GO TO 100
106 IF(ICODE(10)-8HVIBRADIF)108,107
107 CALL VIBRADIF
   GO TO 100
108 IF(ICODE(10)-8HSPORDIF2)110,109
109 JUMP=1
   CALL SPORDIF2
   GO TO 100
110 CONTINUE
   2 FORMAT (I1,7X,2R1,X,I2,2X,R1,3X,F13.4,7X,F4.2,29X,A8)
   50 FORMAT(*1THE FOLLOWING FREQUENCIES ARE THE AVERAGE LAMDA DOUBLT F
1REQUENCIES*)
   51 FORMAT(///*          V          LINE          FREQUENCY          WGT*)
   53 FORMAT (*1*)
   54 FORMAT (*0AFTER AVERAGING, THERE ARE*15* FREQUENCIES*/*5*)
101 FORMAT (10A8)
150 FORMAT (9A8)
300 FORMAT(4X,I1*-0*,7X,2R1,3X,I2,*/2*,1X,R1,4X,F10.4,4X,F10.2)
301 FORMAT(I1*-0*5X,2R1,X,I2*/2*R1,3X,F13.4,7X,F4.2)
   END

```

SUBROUTINE LAMDADIF

```

C CALCULATES THE LAMBDA SPLITTINGS AND THE AVERAGE FREQUENCIES
COMMON/1/NU(600),WGT(600),JU(600),JL(600),VU(600),SU(600),SL(600),
1JUMP,N,DSODIFF(100,1),SODIFF(100,3),DWT(100,1),WT(100,3)
COMMON/2/ LAMDA(600),ISUB(600)
COMMON/3/ NCODE(9), IPUN
TYPE INTEGER VU,SU,SL,BRANCH
TYPE REAL NU
PRINT 60
NTOTAL=NLINES=0 & NMAX=N
PRINT 51
DO 50 I=1,N
   II=I+1

```



```

DO 50 J=II,N
IF(VU(I).NE.VU(J)) GO TO 50
IF(JU(I).NE.JU(J).OR.JL(I).NE.JL(J)) GO TO 50
IF(SU(I).NE.SU(J).OR.SL(I).NE.SL(J)) GO TO 50
IF(LAMDA(I).EQ.1R-.OR.LAMDA(I).EQ.1R+) 100,50
100 IF(LAMDA(J).EQ.1R-.OR.LAMDA(J).EQ.1R+) 101,50
101 XLAMDIF=ABS(NU(I)-NU(J))
NU(I)=(NU(I)+NU(J))/2.0
WGT(I)=2*WGT(I)*WGT(J)/(WGT(I)+WGT(J))
LAMDA(I)=1R+
N=N-1
DO 30 L=J,N
LAMDA(L)=LAMDA(L+1)
ISUB(L)=ISUB(L+1)
VU(L)=VU(L+1)
JU(L)=JU(L+1) * JL(L)=JL(L+1)
SU(L)=SU(L+1) * SL(L)=SL(L+1)
NU(L)=NU(L+1)
30 WGT(L)=WGT(L+1)
JLOWER=2*JL(I)-1
BRANCH=JU(I)-JL(I)+40
PRINT 55,VU(I),BRANCH,ISUB(I),JLOWER,NU(I),XLAMDIF,WGT(I)
PUNCH 355,VU(I),BRANCH,ISUB(I),JLOWER,NU(I),XLAMDIF,WGT(I)
NLINES=NLINES+1
NTOTAL=NTOTAL+1
IF(NLINES.GE.50) 52,50
52 PRINT 53
PRINT 51
NLINES=0
50 CONTINUE
PRINT 54, NMAX,NTOTAL
RETURN
51 FORMAT(/// *      V      LINE      FREQUENCY      DIFF,*6X*WT.*)
53 FORMAT (*1*)
54 FORMAT (*0FROM A TOTAL OF *15* FREQUENCIES, A TOTAL OF *15/* LAMD
1A DOUBLETS WERE FOUND*/5*)
55 FORMAT(I5*-0*,5X,2R1,3X,I2,* /2*,F15.4,F10.4,F10.2)
60 FORMAT (*1TABULATED BELOW ARE THE AVERAGE LAMDA DOUBLET FREQUENCIE
1S*/ * AND THE DOUBLET SEPARATION*)
355 FORMAT(I5*-0*,2X,2R1,2X,I2,* /2*,2X,F15.4,F10.4,5X,F10.2)
END

```

SUBROUTINE RTCOMDIF

C CALCULATES THE ROTATIONAL COMBINATION DIFFERENCES

```

COMMON/1/NU(600),WGT(600),JU(600),JL(600),VU(600),SU(600),SL(600),
1JUMP,N,DSODIFF(100,1),SODIFF(100,3)
COMMON/2/ LAMDA(600),ISUB(600)
COMMON/3/ NCODE(9), IPUN
COMMON/4/ TOL
DIMENSION DCDIFF(150,2,1),CDIFF(150,2,3),DWT(150,2,1),WT(150,2,3)
DIMENSION DITEST(150,2,1),ITEST(150,2,3)
TYPE INTEGER V,S,VU,SU,SL
TYPE REAL NU
IN=0

```



```

DO 2000 IA=1,150
DO 2000 IB=1,2
DO 2000 IC=IN,3
2000 ITEST(IA,IB,IC)=1R
PRINT 53
PRINT 51
DO 50 I=1,N
IF(LAMDA(I).NE.1R*.AND.LAMDA(I).NE.1R ) GO TO 50
II=I+1
DO 50 J=II,N
IF(LAMDA(J).NE.1R*.AND.LAMDA(J).NE.1R ) GO TO 50
IF(SU(I).NE.SU(J).OR.SL(I).NE.SL(J)) GO TO 50
IF(VU(I).NE.VU(J)) GO TO 50
IF(JU(I).NE.JU(J)) GO TO 35
V=0
S=SL(I)
IF(JL(I).EQ.JL(J)+1)21,22
21 K=1
CD=NU(J)=NU(I)
WAT=2*WGT(I)*WGT(J)/(WGT(I)+WGT(J))
JJ=JL(J)
GO TO 48
22 IF(JL(I).EQ.JL(J)-1)23,24
23 K=1
CD=NU(I)=NU(J)
WAT=2*WGT(I)*WGT(J)/(WGT(I)+WGT(J))
JJ=JL(I)
GO TO 48
24 IF(JL(I).EQ.JL(J)+2)25,26
25 K=2
CD=NU(J)=NU(I)
WAT=2*WGT(I)*WGT(J)/(WGT(I)+WGT(J))
JJ=JL(J)
GO TO 48
26 IF(JL(I).EQ.JL(J)-2)27,50
27 K=2
CD=NU(I)=NU(J)
WAT=2*WGT(I)*WGT(J)/(WGT(I)+WGT(J))
JJ=JL(I)
GO TO 48
35 IF(JL(I).EQ.JL(J))36,50
36 V=VU(I)
S=SU(I)
IF(JU(I).EQ.JU(J)+1)37,38
37 K=1
CD=NU(I)=NU(J)
WAT=2*WGT(I)*WGT(J)/(WGT(I)+WGT(J))
JJ=JU(J)
GO TO 48
38 IF(JU(I).EQ.JU(J)-1)39,40
39 K=1
CD=NU(J)=NU(I)
WAT=2*WGT(I)*WGT(J)/(WGT(I)+WGT(J))
JJ=JU(I)

```




```

      GO TO 48
40  IF(JU(I),EQ,JU(J)+2)41,42
41  K=2
      CD=NU(I)=NU(J)
      WAT=2*WGT(I)*WGT(J)/(WGT(I)+WGT(J))
      JJ=JU(J)
      GO TO 48
42  IF(JU(I),EQ,JU(J)-2)43,50
43  K=2
      CD=NU(J)=NU(I)
      WAT=2*WGT(I)*WGT(J)/(WGT(I)+WGT(J))
      JJ=JU(I)
48  DELJ=(K-1)*50+JJ
      JLOWER=2*JJ-1
      PRINT 155,S,V,K,JLOWER,CD,WAT,NU(I),NU(J)
155  FORMAT(* *10X,I1,6X,I1,6X,I1,6X,I2,* /2*,3X,F8,4,4X,F4,2,2F10.4)
      IF(WT(DELJ,S,V),NE,0.0) GO TO 49
      WT(DELJ,S,V)=WAT
      CDIFF(DELJ,S,V)=CD
      GO TO 50
49  IF(ABS(CDIFF(DELJ,S,V)-CD),GT,TOL) ITEST(DELJ,S,V)=1R+
      CDIFF(DELJ,S,V)=(CDIFF(DELJ,S,V)*WT(DELJ,S,V)+CD*WAT)/(WT(DELJ,S,V)
1) *WAT)
      WT(DELJ,S,V)=WT(DELJ,S,V)+WAT
50  CONTINUE
      PRINT 53
      PRINT 150, NCODE
      PRINT 51
      NJ=0
      NLINES=0
      NTOTAL=0
      DO 60 S=1,2
      DO 60 V=NJ,3
      DO 60 K=1,2
      DO 60 JJ=1,50
      DELJ=(K-1)*50+JJ
      IF(CDIFF(DELJ,S,V),EQ,0.0) GO TO 60
      JLOWER = 2*JJ-1
      PRINT 55,S,V,K,JLOWER,CDIFF(DELJ,S,V),ITEST(DELJ,S,V),WT(DELJ,S,V)
      IF(.NOT.IPUN) GO TO 1000
      PUNCH355,S,V,K,JLOWER,CDIFF(DELJ,S,V),ITEST(DELJ,S,V),WT(DELJ,S,V)
1000 NLINES=NLINES+1
      NTOTAL=NTOTAL+1
      IF(NLINES.GE,50) 52,60
52  PRINT 53
      NLINES=0
      PRINT 150, NCODE
      PRINT 51
60  CONTINUE
      PRINT 54,N,NTOTAL
51  FORMAT (///10X*SUB*4X*VIB*3X*DELTA*6X*J*7X*COM*7X*WT.* /9X*STATE*
12X*STATE*20X*DIFF.*///)
53  FORMAT (*1*)
54  FORMAT (*0 FROM *I3* INPUT FREQUENCIES A TOTAL OF *I3/* COMBINATI

```



10N DIFFERENCES WERE FOUND*/5*)

```
55 FORMAT(* *10X,I1,6X,I1,6X,I1,6X,I2,*/2*,3X,F8.4,1R1,3X,F4,2)
150 FORMAT (9A8)
355 FORMAT(3I5,I6,*/2*F13.4,1R1,4X,F6.2)
END
```

SUBROUTINE VIBRADIF

```
C CALCULATES THE VIBRATIONAL DIFFERENCES
COMMON/1/NU(600),WGT(600),JU(600),JL(600),VU(600),SU(600),SL(600),
1 JUMP,N,DSQDIFF(100,1),SODIFF(100,3)
COMMON/2/ LAMDA(600),ISUR(600)
COMMON/3/ NCODE(9), IPUN
DIMENSION DVDIFF(200,2,1),VDIFF(200,2,2),DWT(200,2,1),WT(200,2,2)
TYPE REAL NU
TYPE INTEGER VU,SU,SL,S,V
DO 50 I=1,N
IF(LAMDA(I),NE.1R*,AND,LAMDA(I),NE.1R ) GO TO 50
II=I+1
DO 50 J=II,N
IF(LAMDA(J),NE.1R*,AND,LAMDA(J),NE.1R ) GO TO 50
IF(SU(I),NE,SU(J),OR,SL(I),NE,SL(J)) GO TO 50
IF(JU(I),NE,JU(J),OR,JL(I),NE,JL(J)) GO TO 50
K=1
IF(VU(I)=VU(J)) 20,50,21
20 IF(VU(J),EQ,VU(I)+2) K=2
VD=NU(J)-NU(I)
V=VU(I)
JJ=JU(J)
S=SU(I)
GO TO 40
21 IF(VU(I),EQ,VU(J)+2) K=2
VD=NU(I)-NU(J)
V=VU(J)
JJ=JU(J)
S=SU(I)
40 INDEX=(K-1)*100+JJ
WAT=2*WGT(I)*WGT(J)/(WGT(I)+WGT(J))
IF(WT(INDEX,S,V))42,41
41 VDIFF(INDEX,S,V)=VD
WT(INDEX,S,V)=WAT
GO TO 50
42 VDIFF(INDEX,S,V)=(VDIFF(INDEX,S,V)+WT(INDEX,S,V)+VD*WAT)/(WT(INDEX
1,S,V)+WAT)
WT(INDEX,S,V)=WT(INDEX,S,V)+WAT
50 CONTINUE
PRINT 51
NLINE=0
NTOTAL=0
ASSIGN 60 TO NGO
DO 60 S=1,2
DO 60 V=1,3
DO 60 K=1,2
DO 60 JJ=1,50
INDEX=(K-1)*100+JJ
```



```

      IF(VDIFF(INDEX,S,V).EQ.0.0) GO TO 60
      JLOWER=2*JJ-1
      PRINT 55,S,V,K,JLOWER,VDIFF(INDEX,S,V),WT(INDEX,S,V)
      IF(.NOT.IPUN) GO TO 102
      PUNCH 355,S,V,K,JLOWER,VDIFF(INDEX,S,V),WT(INDEX,S,V)
      GO TO 102
60  CONTINUE
      ASSIGN 100 TO NGO
      DO 100 K=1,3
      DO 100 S=1,2
      DO 100 I=1,N
      IF(SU(I).NE.SL(I).OR.SU(I).NE.S) 100,5
5  IF(VU(I).NE.K) 100,10
10 IF(JU(I).NE.JL(I)) 100,15
15 JLOWER=2*JL(I)-1
      V=VU(I)
      PRINT 55,S,V,K,JLOWER,NU(I),WGT(I)
      IF(.NOT.IPUN) GO TO 102
      PUNCH 355,S,V,K,JLOWER,NU(I),WGT(I)
      GO TO 102
100 CONTINUE
      GO TO 105
102 NLINES=NLINES+1
      NTOTAL=NTOTAL+1
      IF(NLINES.GE.50) 52,101
52 PRINT 53
      NLINES=0
      PRINT 150,NCODE
      PRINT 51
101 GO TO NGO
105 PRINT 54,N,NTOTAL
51 FORMAT (///10X*SUB*4X*VIR*3X*DELTA*6X*J*7X*VIB*7X*WT.*/*9X*STATE*
12X*STATE*20X*DIFF.*///)
53 FORMAT (*1*)
54 FORMAT (*0 FROM +I3* INPUT FREQUENCIES A TOTAL OF +I3/* VIBRATIONA
1L DIFFERENCES WERE FOUND+/*5*)
55 FORMAT (* *10X,I1,6X,I1,6X,I1,6X,I2,*/*2*,2X,F9.4,4X,F4.2)
150 FORMAT (9A8)
355 FORMAT(4I5,*/*2*7X,F10.4,F10.2)
      END

```

SUBROUTINE SPORDIF1

```

C  CALCULATES THE SPIN-ORBIT DIFFERENCES FOR THE V=0 STATE
      COMMON/1/NU(600),WGT(600),JU(600),JL(600),VU(600),SU(600),SL(600),
1JUMP,N,DSODIFF(100,1),SODIFF(100,3),DWT(100,1),WT(100,3)
      COMMON/2/ LAMDA(600),ISUB(600)
      COMMON/3/ NCODE(9), IPUN
      COMMON/4/ TOL
      DIMENSION DITEST(100,1), ITEST(100,3)
      TYPE INTEGER V,S,VU,SU,SL
      TYPE REAL NU
      IN=0
      DO 2000 IA=1,100
      DO 2000 IB=IN,3

```



```

2000 ITEST(IA,IR)=1R
PRINT 53
PRINT 51
DO 50 I=1,N
IF(LAMDA(I).NE.1R*.AND.LAMDA(I).NE.1R ) GO TO 50
II=I+1
DO 50 J=I,N
IF(LAMDA(J).NE.1R*.AND.LAMDA(J).NE.1R ) GO TO 50
IF(JU(I).NE.JU(J).OR.JL(I).NE.JL(J)) GO TO 50
IF(SU(I).NE.SU(J)) GO TO 35
IF(SL(I).EQ.SL(J)) GO TO 50
JJ=JL(I)
V=0
IF(SL(I).EQ.1) 40,41
35 IF(SL(I).NE.SL(J)) GO TO 50
V=VU(I)
JJ=JU(I)
IF(SU(I).EQ.2) 40,41
40 SOD=NU(I)-NU(J)
GO TO 42
41 SOD=NU(J)-NU(I)
42 WAT=2*WGT(I)*WGT(J)/(WGT(I)+WGT(J))
JM=2*JJ-1
PRINT 155, V,JM,SOD,WAT,NU(I),NU(J)
155 FORMAT(2I5/,2*7X,F10.4,10X,F10.2,2F10.4)
IF(WT(JJ,V).NE.0.0) 45,43
43 WT(JJ,V)=WAT
SODIFF(JJ,V)=SOD
GO TO 50
45 IF(ABS(SODIFF(JJ,V)-SOD).GT.10L) ITEST(JJ,V)=1R+
SODIFF(JJ,V)=(SODIFF(JJ,V)+WT(JJ,V)+SOD*WAT)/(WT(JJ,V)+WAT)
WT(JJ,V)=WT(JJ,V)+WAT
50 CONTINUE
IF(JUMP) RETURN
PRINT 53
PRINT 150,NCODE
PRINT 51
NJ=0
NLINES=0
NTOTAL=0
DO 60 V=NJ,1
DO 60 JJ=1,50
IF(SODIFF(JJ,V).EQ.0.0) GO TO 60
JM=2*JJ-1
PRINT 55,V,JM,SODIFF(JJ,V),ITEST(JJ,V),WT(JJ,V)
IF(.NOT. IPUN) GO TO 1000
PUNCH355,V,JM,SODIFF(JJ,V),ITEST(JJ,V),WT(JJ,V)
1000 NLINES=NLINES+1
NTOTAL=NTOTAL+1
IF(NLINES.GE.50) 52,60
52 PRINT 53
NLINES=0
PRINT 150,NCODE
PRINT 51

```




```

60 CONTINUE
   PRINT 54,N,NTOTAL
51 FORMAT (///14X*V+9X*J*8X*SPIN ORBIT*8X*WEIGHT*/33X*DIFFERENCE*///)
53 FORMAT (*1*)
54 FORMAT (*0 FROM *I3* INPUT FREQUENCIES A TOTAL OF *I3/* SPIN ORBIT
   DIFFERENCES FOR THE V=0 AND V=1*/ * STATES WERE FOUND*/ *5*)
55 FORMAT (* *13X,I1,7X,I2,* /2*,8X,F8.4,R1,9X,F4.2)
150 FORMAT (9AR)
355 FORMAT (2I5*/2*7X,F10.4,R1,9X,F10.2)
END

```

SUBROUTINE SPORDIF2

```

C CALCULATES THE SPIN-ORBIT DIFFERENCE FOR EXCITED V-STATES
COMMON/1/NU(600),WGT(600),JU(600),JL(600),VU(600),SU(600),SL(600),
1JUMP,N,DSODIFF(100,1),SODIFF(100,3),DWT(100,1),WT(100,3)
COMMON/2/ LAMDA(600),ISUB(600)
COMMON/3/ NCODE(9), IPUN
DIMENSION DWET(100,1),WET(100,3)
TYPE REAL NU
TYPE INTEGER V,S,VU,SU,SL
CALL SPORDIF1
DO 50 I=1,N
  IF(LAMDA(I).NE.1R*.AND.LAMDA(I).NE.1R ) GO TO 50
  II=I+1
  DO 50 J=II,N
    IF(LAMDA(J).NE.1R*.AND.LAMDA(J).NE.1R ) GO TO 50
    IF(SU(I).EQ.SU(J).OR.SL(I).EQ.SL(J).OR.SU(I).NE.SL(I)) 50,22
22 IF(JU(I).NE.JU(J).OR.JL(I).NE.JL(J)) 50,23
23 IF(VU(I).EQ.VU(J).AND.VU(I).NE.1) 24,50
24 IF(VU(I).EQ.2) 25,26
25 V=2
    GO TO 27
26 V=3
27 JJ=JU(I)
    IF(SU(I).EQ.2) 28,29
28 SOD=NU(I)-NU(J)+SODIFF(JJ,0)
    GO TO 40
29 SOD=NU(J)-NU(I)+SODIFF(JJ,0)
40 WAT=3*WGT(I)*WGT(J)*WT(JJ,0)/(WGT(I)+WGT(J)+WT(JJ,0))
    IF(WET(JJ,V).NE.0.0) 45,43
43 WET(JJ,V)=WAT
    SODIFF(JJ,V)=SOD
    GO TO 50
45 SODIFF(JJ,V)=(SODIFF(JJ,V)+WET(JJ,V)+SOD*WAT)/(WET(JJ,V)+WAT)
    WET(JJ,V)=WET(JJ,V)+WAT
50 CONTINUE
   PRINT 51
   NLINES=0
   NTOTAL=0
   DO 60 V=2,3
     DO 60 JJ=1,50
       IF(SODIFF(JJ,V).EQ.0.0) GO TO 60
       JM=2*JJ-1
       IF(SODIFF(JJ,V).LT.0.0) 56,57

```



```

54 PRINT 75, V, JM
   GO TO 102
57 PRINT 55, V, JM, SODIFF(JJ,V), WET(JJ,V)
   IF(.NOT.IPUN) GO TO 102
   PUNCH 355,V,JM,SODIFF(JJ,V),WET(JJ,V)
102 NLINES=NLINES+1
   NTOTAL=NTOTAL+1
   IF(NLINES.GE.50) 52,60
52 PRINT 53
   NLINES=0
   PRINT 150,NCODE
   PRINT 51
60 CONTINUE
   PRINT 54,N,NTOTAL
51 FORMAT (///14X*V*9X*J*8X*SPIN ORBIT*8X*WEIGHT*/33X*DIFFERENCE*///)
53 FORMAT (*1*)
54 FORMAT (*0 FROM *I3* INPUT FREQUENCIES A TOTAL OF *I3/* SPIN ORBIT
  1T DIFFERENCES FOR THE V=2 AND V=3*/ STATES WERE FOUND*/*5*)
55 FORMAT (* *13X,I1,7X,I2,*/*2*,8X,F8.4,10X,F4.2)
75 FORMAT (* *13X,I1,7X,I2,*/*2 SPIN ORBIT DIFFERENCE IS NEGATIVE*)
150 FORMAT (9A8)
355 FORMAT(2I5,*/*2*7X,F10.4,10X,F10.2)
   END

```


- C. ROTCONS
- D. ALLFIT
- E. LAMCON
- F. STEPFIT

Programs in sections C, D, and E use subroutine STEPFIT (Section F) which is a least squares routine written by M. A. Efroymsen (75). ROTCONS fits rotational combination differences, ALLFIT fits frequencies and LAMCON fits Λ -doublet splittings. All three have essentially the same input and thus a general description follows.

STRUCTURE OF DATA DECKS

I. Constants cards

CONSTANT in cols. 73-80 indicates that the following cards have initial or fixed values of the constants.

1. Heading cards: Cols. 1-72 are read and printed until END HEAD in cols. 73-80 is encountered.
2. Values of the constants: Read in cols. 1-20 in the following orders:

ROTCONS: $B_{01}, B_{02}, D_{01}, D_{02}, H_{01}, H_{02}, \alpha_1, \alpha_2, \beta_1, \beta_2, \gamma_1, \gamma_2,$
 $H'_0, \gamma'.$

ALLFIT: $\Delta G(1), H'_0, \gamma', Q_0, \chi, B_{01}, B_{02}, D_{01}, D_{02}, \alpha_1, \alpha_2, \beta_1, \beta_2,$
 $H_{01}, H_{02}, \gamma_1, \gamma_2.$

LAMCON: $p_\Lambda, q_\Lambda.$

II. Data cards

NEW DATA in cols. 73-80 indicates that the following cards contain information to be fit. The formats are as follows:

<u>Cols.</u>	<u>Field</u>	<u>Variable</u>
1. <u>ROTCONS</u>		
1-5	I	Substate of difference.
6-10	I	Vibration level of difference.
11-15	I	ΔJ
16-21	I	2J
25-36	F	Combination difference.
41-46	F	Weight.
2. <u>ALLFIT</u>		
1	I	Upper vibrational state.
9	R	Branch (P, Q, or R).
10	R	Subbranch (1, 2, H, L).
12-13	I	2J
20-33	F	Frequency
41-44	F	Weight
3. <u>LAMCON</u>		
10	R	Branch (P, Q, or R).
11	R	Subbranch (1, 2, H, L)
14-15	I	2J
34-49	F	Λ -doublet splitting
50-59	F	Weight

"END DATA" in cols. 73-80 signals the end of data.

III. Information card

<u>Col.</u>	<u>Field</u>	<u>Function</u>
1-5	I	$\neq 0$ indicates statistical information from STEPFIT is desired.



<u>Col.</u>	<u>Field</u>	<u>Function</u>
6-10	I	Number of data points to be deleted if subsequent fits warrant it.
20-29	F	If the weighted observed minus predicted value is larger than this, the line is deleted and the fit is repeated. The largest deviation is deleted first.
30-39	F	If the value of the diagonal element of the inverse matrix is less than this number, that variable is not included in the fit.
40-49	F	Value of the minimum change in the value of a variable before it will be entered. Preset to 10^{-8} .
50-59	F	Value of the minimum change in the value of a variable before it will be removed.
70-72	I	$\neq 0$ indicates a punch output of the fit is desired.
73-80	A	Ident field for the molecule.

IV. Option card

This card controls which variables will be entered in the fit. The order of the variables for each program is as given in I above. Starting from column one, a non-zero punch in the column corresponding to a particular variable will cause it to be entered in the fit.

V. Heading cards

These cards are read and printed until END HEAD is encountered in cols. 73-80.



VI. Control card

This card is read and depending upon the content of cols. 73-80, control is returned to the appropriate section:

CONSTANT → Section I

NEW DATA → Section II

blank → Section IV (Option card data should appear)

LAST FIT → Ends execution

The listings of ROTCONS, ALLFIT, LAMCON and STEPFIT follow.

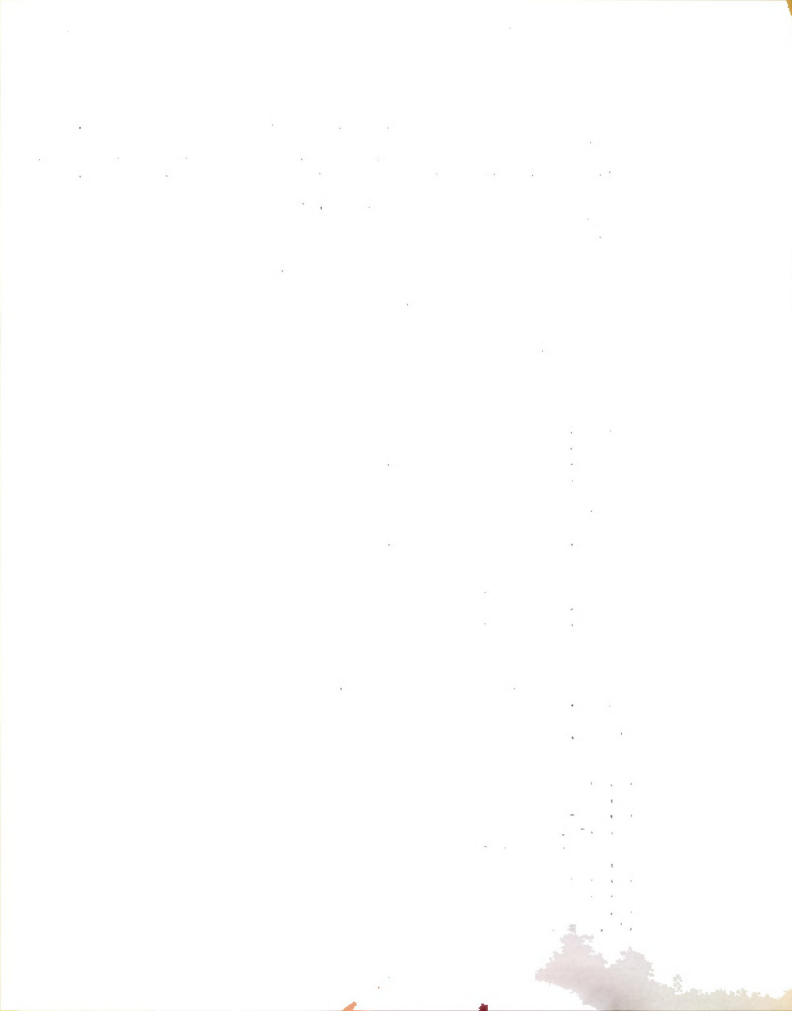


C, ROTCONS

```

PROGRAM ROTCONS
COMMON/1/NODATA,NOVMI,AVEWHT,STDY,NOSTEP,N,WTN,FREQPRD,YPRED,DEV,
1DATA(20,500)
COMMON/2/FOBS(500),FCALC(500),WT(500),NK(17),INFO,INDATA,NDELMAX,X
1DEVMAX,N1(25),MOL,CON(17,500),IH(10),SS(200),VV(500),KK(500),JJ(50
20),NUMCON,ISTATE
COMMON/3/ NOVAR,JUMP,CONST(20),EFIN,EFOUT
COMMON/5/ TOL
COMMON/10/ IPUNCH
COMMON/C/ NAME(30)
DATA(NAME=3HB01,3HB02,3HD01,3HD02,3HH01,3HH02,6HALPHA1,6HALPHA2,
15HBETA1,5HBETA2,6HGAMMA1,6HGAMMA2,3HH02,6HGAMMA2)
EXTERNAL ROTCONS1,ROTCONS2,ROTCONS3
TYPE INTEGER SS,VV
TYPE REAL J
U(J,P)=(J+P+.5)**2
F(J)=(J+.5)**2
NUMCON=14 $ ISTATE=0
1000 JUMP=0
    READ 50,IH
    100 IF(IH(10),EQ.8HLAST FIT) 900,110
    110 IF(IH(10),EQ.8HEND DATA) 365,120
    120 IF(IH(10),EQ.8HCONSTANT) 150,130
    130 IF(IH(10),EQ.8HNEW DATA)300,900
    150 JUMP=1
    160 READ 50,IH
        PRINT 50,(IH(I),I=1,9)
        IF(IH(10),EQ.8HEND HEAD) 200,160
    200 PRINT 53
        J1=1
    210 READ 220,CONST(J1),IH(10)
        IF(IH(10),NE.8H ) 100,230
    230 PRINT 240,NAME(J1),CONST(J1)
        J1=J1+1
        GO TO 210
    300 M=1
    350 READ 355, SS(M),VV(M),KK(M),JJ(M),FOBS(M),WT(M),IH(10)
        IF(IH(10),NE.8H ) 100,360
    360 INDATA=M
        J=JJ(M)/2,
        P=KK(M)
        GO TO (1200,1300) SS(M)
1200 CON(1,M)=U(J,P)*F(J)
        CON(2,M)=0,
        CON(3,M)=-(U(J,P)**2-F(J)**2)
        CON(4,M)=0,
        CON(5,M)=U(J,P)**3-F(J)**3
        CON(6,M)=0,
        CON(7,M)=-CON(1,M)*VV(M)
        CON(8,M)=0,
        CON(9,M)=CON(3,M)*VV(M)
        CON(10,M)=0,

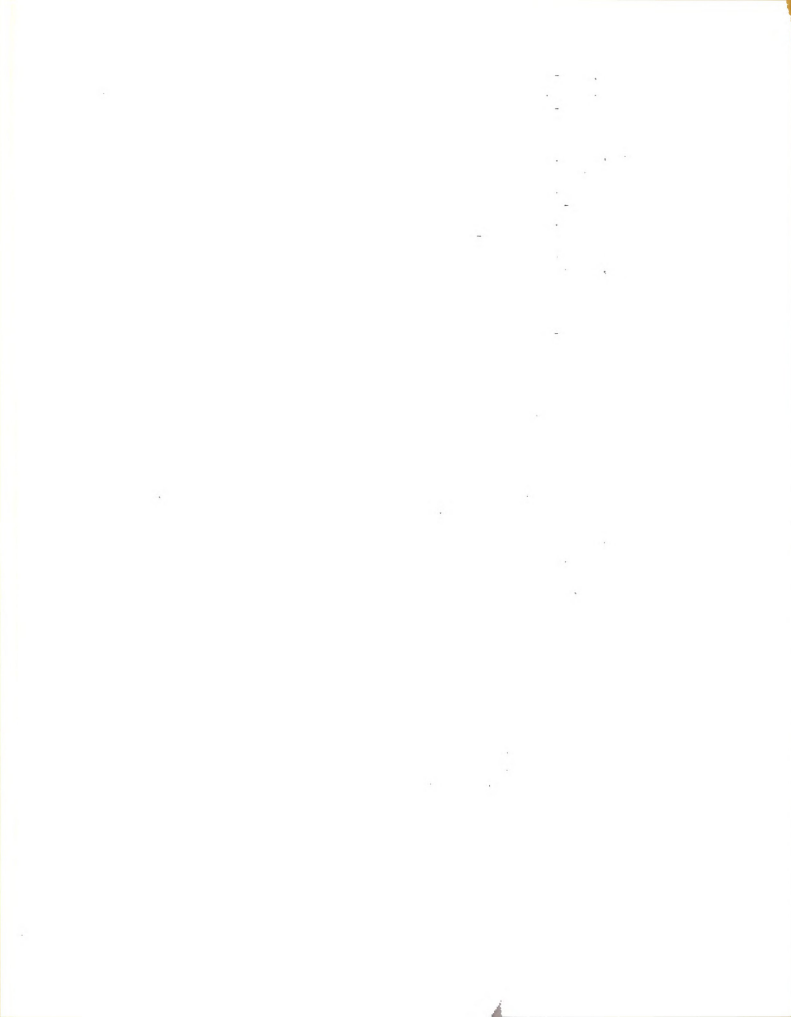
```



```

CON(11,M)=-CON(5,M)*VV(M)
CON(12,M)=0,
CON(13,M)=-CON(5,M)
CON(14,M)=-CON(11,M)
GO TO 1400
1300 CON(1,M)=0,
CON(2,M)=U(J,P)-F(J)
CON(3,M)=0,
CON(4,M)=-(U(J,P)**2-F(J)**2)
CON(5,M)=0,
CON(6,M)=U(J,P)**3-F(J)**3
CON(7,M)=0,
CON(8,M)=-CON(2,M)*VV(M)
CON(9,M)=0,
CON(10,M)=CON(4,M)*VV(M)
CON(11,M)=0,
CON(12,M)=-CON(6,M)*VV(M)
CON(13,M)=CON(6,M)
CON(14,M)=CON(12,M)
1400 CONTINUE
FCALC(M)=0,
IF(JUMP) 380,390
380 DO 385 L=1,14
385 FCALC(M)=FCALC(M)+CONST(L)*CON(L,M)
390 M=M+1
GO TO 350
365 READ 40, INFO,NDELMAX,XDEVMAX,TOL,EFIN,EFOUT,IPUNCH,MOL
40 FORMAT(2I5,9X,4F10,10X,I3,A8)
20 READ 45, (NK(I),I=1,14),IH(10)
45 FORMAT(14I1,58X,A8)
IF(IH(10),NE.8H ) GO TO 100
25 READ 50, IH
PRINT 50, (IH(M),M=1,9)
IF(IH(10),NE.8HEND HEAD) GO TO 25
CALL STEP FIT(ROTCONS1,ROTCONS2,ROTCONS3)
GO TO 20
900 CONTINUE
PRINT 54
50 FORMAT (10A8)
51 FORMAT (*1*/ )
53 FORMAT (///)
54 FORMAT (*5*)
220 FORMAT (F20,52X,A8)
240 FORMAT (A20,F30,10)
355 FORMAT (3I5,16,3X,F12,4,5X,F6.1,25X,A8)
END

```

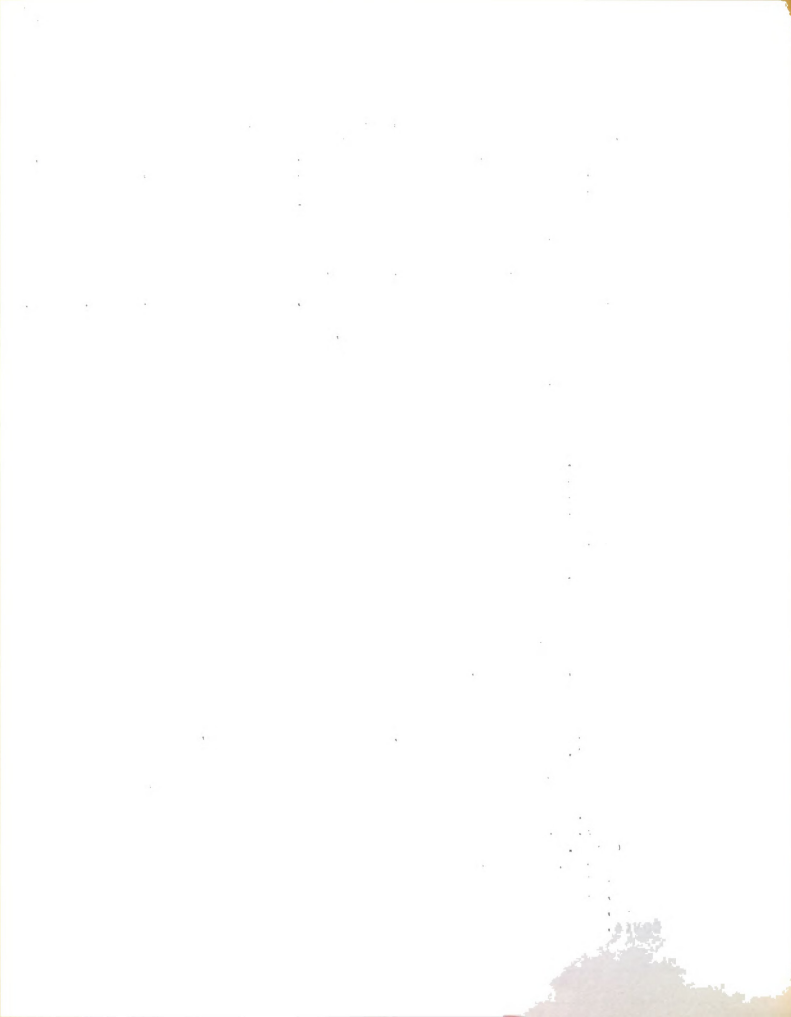



D, ALLFIT

```

PROGRAM ALLFIT
COMMON/1/NODATA,NOVMI,AVEWHT,STDY,NOSTEP,N,WTN,FREQPRD,YPRED,DEV,
1DATA(20,500)
COMMON/2/FOBS(500),FCALC(500),WT(500),NK(17),INFO,INDATA,NDELMAX,
1XDEVMAX,N1(25),MOL,CON(17,500),IH(10),SS(500),VV(500),KK(500),
2JJ(500),NUMCON,ISTATE
COMMON/3/ NOVAR,JUMP,CONST(20),EFIN,EFOUT
COMMON/5/ TOL
COMMON/10/ IPUNCH
COMMON/C/ NAME(30)
DATA(IV1=1,0,0),(IV2=0,1,0),(IV3=0,0,1)
DATA(NAME=7HDELTA1,3HH02,6HGAMMA2,3HAA0,3HCH1,3HB01,
13HB02,3HD01,3HD02,7HALPHA 1,7HALPHA 2,5HBETA1,5HBETA2,3HH01,3HH02,
26HGAMMA1,6HGAMMA2)
DIMENSION IV1(3),IV2(3),IV3(3)
EXTERNAL FITALL1,FITALL2,FITALL3
TYPE INTEGER BRANCH,VV,SS
TYPE REAL J,NU,K
U(J,K)=(J+K+.5)**2
F(J)=(J+.5)**2
JUMP=0 $ NUMCON=17 $ ISTATE=0
1000 READ 50, IH
100 IF(IH(10),EQ.8HLAST FIT) 900,110
110 IF(IH(10),EQ.8HEND DATA) 365,120
120 IF(IH(10),EQ.8HCONSTANT) 150,130
130 IF(IH(10),EQ.8HNEW DATA) 300,900
150 JUMP=1
160 READ 50,IH
PRINT 50, (IH(I),I=1,9)
IF(IH(10),EQ.8HEND HEAD) 200,160
200 PRINT 53
J1=1
210 READ 220, CONST(J1),IH(10)
IF(IH(10),NE.8H ) GO TO 100
IF(CONST(J1),EQ.0,0) GO TO 230
PRINT 240, NAME(J1),CONST(J1)
230 J1=J1+1
GO TO 210
300 N=1
310 READ 355,VV(N),BRANCH,SS(N),JJ(N),FOBS(N),WT(N),IH(10)
IF(IH(10),NE.8H ) GO TO 100
INDATA=N
KK(N)=BRANCH-1RQ
K=KK(N)
IF(SS(N),EQ,1RL)SS(N)=4
IF(SS(N),EQ,1RH)SS(N)=3
J=JJ(N)/2,
GO TO (410,420,430,440) SS(N)
410 CON(1,N)=IV1(VV(N))
CON(4,N)=0,
CON(5,N)=VV(N)/2,
CON(6,N)=U(J,K)-F(J)

```



```

CON(7,N)=0,
CON(8,N)=-(U(J,K)**2)+(F(J)**2)
CON(9,N)=0,
CON(10,N)=-(U(J,K)+,5)*VV(N)
CON(11,N)=-VV(N)/2,
CON(12,N)=-(U(J,K)**2+,5)*VV(N)
CON(13,N)=-VV(N)/2,
CON(14,N)=(U(J,K)**3)-(F(J)**3)
CON(15,N)=0,
CON(16,N)=-(U(J,K)**3)*VV(N)
CON(17,N)=0,
CON(2,N)=-CON(14,N)
CON(3,N)=-CON(16,N)
GO TO 450
420 CON(1,N)=IV1(VV(N))
CON(4,N)=0,
CON(5,N)=-VV(N)/2,
CON(6,N)=0,
CON(7,N)=U(J,K)-F(J)
CON(8,N)=0,
CON(9,N)=-(U(J,K)**2)+(F(J)**2)
CON(10,N)=VV(N)/2,
CON(11,N)=-(U(J,K)-,5)*VV(N)
CON(12,N)=-VV(N)/2,
CON(13,N)=-(U(J,K)**2+,5)*VV(N)
CON(14,N)=0,
CON(15,N)=(U(J,K)**3)-(F(J)**3)
CON(16,N)=0,
CON(17,N)=-(U(J,K)**3)*VV(N)
CON(2,N)=CON(15,N)
CON(3,N)=CON(17,N)
GO TO 450
430 CON(1,N)=IV1(VV(N))
CON(4,N)=1,
CON(5,N)=-VV(N)/2,
CON(6,N)=-F(J)
CON(7,N)=U(J,K)
CON(8,N)=F(J)**2
CON(9,N)=-(U(J,K)**2)
CON(10,N)=VV(N)/2,
CON(11,N)=-(U(J,K)-,5)*VV(N)
CON(12,N)=-VV(N)/2,
CON(13,N)=-(U(J,K)**2+,5)*VV(N)
CON(14,N)=-(F(J)**3)
CON(15,N)=U(J,K)**3
CON(16,N)=0,
CON(17,N)=-(U(J,K)**3)*VV(N)
CON(2,N)=CON(15,N)-CON(14,N)
CON(3,N)=CON(17,N)
GO TO 450
440 CON(1,N)=IV1(VV(N))
CON(4,N)=-1,
CON(5,N)=VV(N)/2,
CON(6,N)=U(J,K)

```



```

CON(7,N)=- F(J)
CON(8,N)=- (U(J,K)**2)
CON(9,N)=F(J)**2
CON(10,N)=- (U(J,K)+.5)*VV(N)
CON(11,N)=-VV(N)/2,
CON(12,N)=- (U(J,K)**2+.5)*VV(N)
CON(13,N)=-VV(N)/2,
CON(14,N)=U(J,K)**3
CON(15,N)=- (F(J)**3)
CON(16,N)=- (U(J,K)**3)*VV(N)
CON(17,N)=0,
CON(2,N)=CON(15,N)-CON(14,N)
CON(3,N)=-CON(16,N)
450 CONTINUE
FCALC(N)=0,
IF(JUMP) 380,390
380 DO 385 LL=1,NUMCON
385 FCALC(N)=FCALC(N)+CONST(LL)*CON(LL,N)
390 N=N+1
GO TO 310
365 READ 40, INFO,NDELMAX,XDEVMAX,TOL,EFIN,EFOUT,IPUNCH,MOL
20 READ 45, (NK(I),I=1,17),IH(10)
IF(IH(10),NE.8H ) GO TO 100
25 READ 50, IH
PRINT 50, (IH(M),M=1,9)
IF(IH(10),NE.8HEND HEAD) GO TO 25
CALL STEP FIT(FITALL1,FITALL2,FITALL3)
GO TO 20
900 CONTINUE
40 FORMAT(2I5,9X,4F10,10X,I3,A8)
45 FORMAT (17I1,55X,A8)
50 FORMAT(10A8)
53 FORMAT(*-*)
220 FORMAT(F20,52X,A8)
240 FORMAT(A20,F30,10)
355 FORMAT(I1,7X,2R1,X,I2,6X,F13,4,7X,F4,2,29X,A8)
END

```

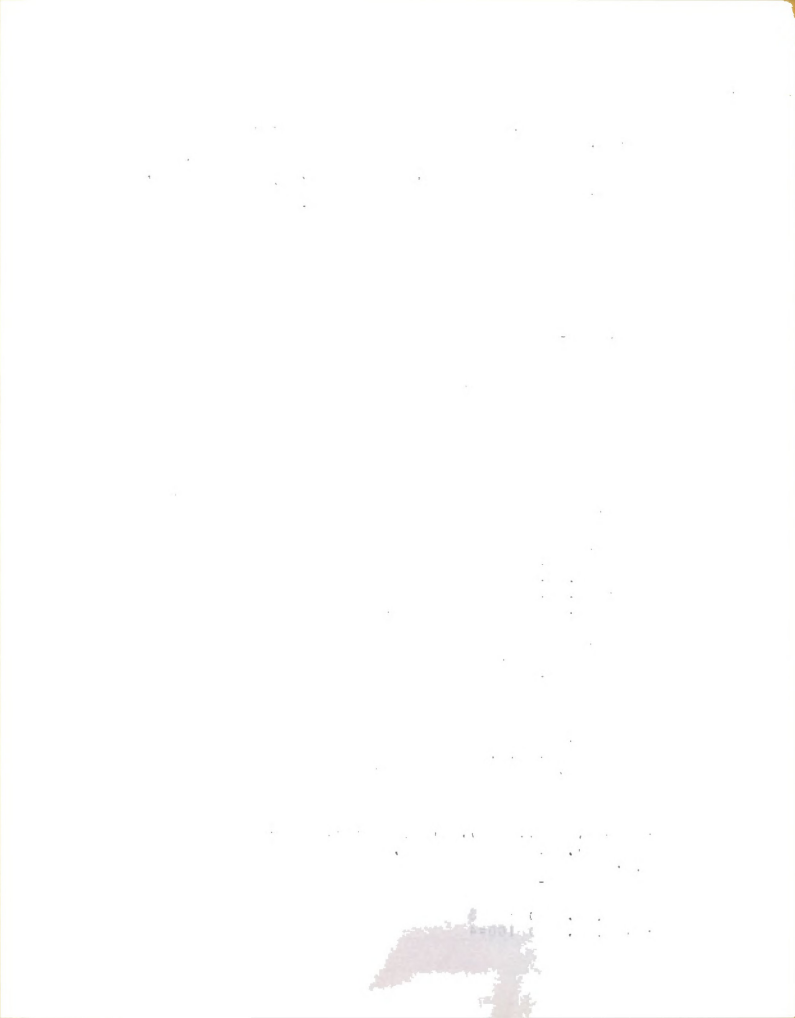


E. LAMCON

```

PROGRAM LAMCON
COMMON/1/NODATA,NOVMI,AVEWHT,STDY,NOSTEP,N,WTN,FREQPRD,YPRED,DEV,
1DATA(20,500)
COMMON/2/FOBS(500),FCALC(500),WT(500),NK(17),INFO,INDATA,NDELMAX,
1XDEVMAX,N1(25),MOL,CON(17,500),IH(10),SS(500),VV(500),KK(500),
2JJ(500),NUMCON,ISTATE
COMMON/3/ NOVAR,JUMP,CONST(20),EFIN,EFDUT
COMMON/5/ TOL
COMMON/10/ IPUNCH
COMMON/C/ NAME(30)
DATA(NAME=2HPL,2HQL)
EXTERNAL LAMCON1,LAMCON2,LAMCON3
TYPE INTEGER BRANCH,SS
TYPE REAL J
U(J)=(J**2-.25)*(J+1,5)
F(J)=(J*,50)
ISTATE=0 $ NUMCON=2 $ JUMP=0
READ 9000, A0,A1,B01,B02,B11,B12
9000 FORMAT(6F10)
XL01=A0/B01
XXL01=XL01*XL01
XL02=A0/B02
XXL02=XL02*XL02
XL11=A1/B11
XXL11=XL11*XL11
XL12=A1/B12
XXL12=XL12*XL12
1000 READ 50,IH
100 IF(IH(10),EQ.8HLAST FIT) 900,110
110 IF(IH(10),EQ.8HEND DATA) 365,120
120 IF(IH(10),EQ.8HCONSTANT) 150,130
130 IF(IH(10),EQ.8HNEW DATA) 300,900
150 JUMP=1
160 READ 50, IH
PRINT 50, (IH(I),I=1,9)
IF(IH(10),EQ.8HEND HEAD) 200,160
200 PRINT 53
J1=1
210 READ 220,CONST(J1),IH(10)
IF(IH(10),NE.8H ) 100,230
230 IF(CONST(J1).EQ.0,0) GO TO 235
PRINT 240 , NAME(J1),CONST(J1)
235 J1=J1+1
GO TO 210
300 M=1
1350 READ 301,SS(M),KK(M),JJ(M),FOBS(M),WT(M),IH(10)
IF(IH(10),NE.8H )100,360
360 J=,5*JJ(M)
BRANCH=SS(M)-1R0
IGO=KK(M)
IF(IGO,EQ,1RH) IGO=3
IF(IGO,EQ,1RL) IGO=4

```

```

GO TO (1370,1380,370,380) IGO
370 GO TO (372,374,376) BRANCH
372 CON(1,M)=2.*F(J)-2.*U(J-1)/XXL12=2.*U(J)/XXL01
CON(2,M)=-(4.*U(J-1)/XL12+4.*U(J)/XL01)
GO TO 390
374 CON(1,M)=-(2.*F(J)+2.*U(J)/XXL12=2.*U(J)/XXL01)
CON(2,M)=-(1./XL12-1./XL01)+4.*U(J)
FOBS(M)=-FOBS(M)
GO TO 390
376 CON(1,M)=2.*F(J)-2.*U(J+1)/XXL12=2.*U(J)/XXL01
CON(2,M)=-(4.*U(J+1)/XL12+4.*U(J)/XL01)
GO TO 390
380 GO TO (382,384,386) BRANCH
382 CON(1,M)=-(2.*F(J)-2.*U(J-1)/XXL11=2.*U(J)/XXL02)
CON(2,M)=4.*U(J-1)/XL11+4.*U(J)/XL02
FOBS(M)=-FOBS(M)
GO TO 390
384 CON(1,M)=-(2.*F(J)+2.*U(J)/XXL02=2.*U(J)/XXL11)
CON(2,M)=(1./XL11-1./XL02)+4.*U(J)
FOBS(M)=-FOBS(M)
GO TO 390
386 CON(1,M)=-(2.*F(J)-2.*U(J+1)/XXL11=2.*U(J)/XXL02)
CON(2,M)=4.*U(J+1)/XL11+4.*U(J)/XL02
FOBS(M)=-FOBS(M)
GO TO 390
1370 GO TO (1372,1374,1376) BRANCH
1372 CON(1,M)=2.+2.*U(J-1)/XXL11+2.*U(J)/XXL01
CON(2,M)=4.*U(J-1)/XL11+4.*U(J)/XL01
GO TO 390
1374 CON(1,M)=-4.*F(J)+2.*U(J)/XXL11+2.*U(J)/XXL01
CON(2,M)=4.*(1./XL11+1./XL01)*U(J)
FOBS(M)=-FOBS(M)
GO TO 390
1376 CON(1,M)=-2.+2.*U(J+1)/XXL11=2.*U(J)/XXL01
CON(2,M)=4.*(U(J+1)/XL11+U(J)/XL01)
FOBS(M)=-FOBS(M)
GO TO 390
1380 GO TO (1382,1384,1386) BRANCH
1382 CON(1,M)=-2.*U(J-1)/XXL12+2.*U(J)/XXL02
CON(2,M)=-4.*U(J-1)/XL12+4.*U(J)/XL02
GO TO 390
1384 CON(1,M)=-1./XXL12+1./XXL02+2.*U(J)
CON(2,M)=-1./XL12+1./XL02+4.*U(J)
FOBS(M)=-FOBS(M)
GO TO 390
1386 CON(1,M)=-2.*U(J+1)/XXL12+2.*U(J)/XXL02
CON(2,M)=-4.*U(J+1)/XL12+4.*U(J)/XL02
FOBS(M)=-FOBS(M)
390 FCALC(M)=0.0
IF(JUMP) 400,500
400 DO 70 K=1,NUMCON
70 FCALC(M)=FCALC(M)+CON(K,M)*CONST(K)
500 M=M+1
GO TO 1350

```

the same time, the *Journal of the American Medical Association* (JAMA) published a series of articles that highlighted the importance of medical research in the treatment of cancer. These articles, which were part of a larger report titled "The National Cancer Institute's Program for the Control and Prevention of Cancer," emphasized the need for a coordinated effort between the government and the medical community to combat the disease. The report also outlined the various research programs that were being funded by the NCI, including studies on the causes of cancer, the development of new treatments, and the improvement of diagnostic techniques.

One of the key findings of the report was that cancer was a complex disease that required a multidisciplinary approach to its treatment. This meant that researchers from different fields, such as biology, chemistry, and physics, had to work together to understand the underlying mechanisms of the disease. The report also stressed the importance of clinical trials, which were essential for testing new treatments and determining their effectiveness.

In addition to the NCI's research programs, the report also discussed the role of the medical community in the fight against cancer. It emphasized the need for doctors to stay up-to-date on the latest research and to work closely with researchers to develop new treatments. The report also highlighted the importance of patient education, which was essential for helping patients understand their condition and make informed decisions about their treatment.

Overall, the report provided a comprehensive overview of the NCI's research programs and the role of the medical community in the fight against cancer. It also outlined the various challenges that researchers and doctors faced in the early 1970s and provided suggestions for how to overcome these challenges.

The report was a landmark document in the history of cancer research, as it provided a clear vision of the future of the field and outlined the steps that needed to be taken to achieve this vision. It also helped to raise public awareness of the importance of cancer research and the need for continued funding for these programs. The report's findings and recommendations have had a lasting impact on the field of cancer research, and its principles continue to guide researchers and doctors today.

One of the key challenges that researchers and doctors faced in the early 1970s was the lack of a coordinated effort between the government and the medical community. At that time, the NCI was still in its infancy, and its research programs were limited in scope. Additionally, the medical community was largely unaware of the latest research in cancer, and there was a lack of communication between researchers and doctors. The report addressed these challenges by outlining the need for a coordinated effort and by providing suggestions for how to improve communication and collaboration between the government and the medical community.

```
365 INDATA=M-1
30 READ 40, INFO,NDELMAX,XDEVMAX,TOL,EFIN,EFOUT,IPUNCH,MOL
340 READ 45,(NK(I),I=1,2),IH(10)
    IF(IH(10),NE.8H          )100,21
21 PRINT 51
20 READ 50,IH
    PRINT 50,(IH(I),I=1,9)
    IF(IH(10),EQ.8HEND HEAD) 350,20
350 CALL STEP FIT (LAMCON1,LAMCON2,LAMCON3)
    GO TO 340
900 CONTINUE
    PRINT 54
40 FORMAT(2I5,9X,4F10,10X,I3,A8)
45 FORMAT( 2I1,70X,A8)
50 FORMAT(10A8)
51 FORMAT(*1*/ )
53 FORMAT(*** )
54 FORMAT(*5* )
220 FORMAT(F20,52X,A8)
240 FORMAT(A20,F30,10)
301 FORMAT(9X,2R1,2X,I2,19X,F15,4,F10,13X,A8)
    END
```


F. STEPFIT

```

SUBROUTINE STEP FIT(HEAD1,HEAD2,OUTPUT)
  COMMON/1/NODATA,NOVMI,AVEWHT,STDY,NOSTEP,N,WTN,FREQPRD,YPRED,DEV,
1 DATA(20,500)
  COMMON/2/FOBS(500),FCALC(500),WT(500),NK(17),INFO,INDATA,NDELMAX,
1 XDEVMAX,N1(25),MCL,CON(17,500),IH(10),SS(500),VV(500),KK(500),
2 JJ(500),NUMCON,ISTATE
  COMMON/3/ NOVAR,JUMP,CONST(20),EFIN,EFOUT
  COMMON/C/ NAME(30)
  COMMON/5/ TOL
  COMMON/10/ IPUNCH
  DIMENSION VECTOR(20,20),INDEX(20),SIGMA(20),COEN(20),SIGMCO(20),
1 NOTIN(20),NUSE(500)
  DIMENSION XCONST(20)
  TYPE INTEGER SS,VV
  TYPE DOUBLE VECTOR,SIGMA,COEN,SIGMCO,SIGY,DEFR,VAR
  IF(.NOT.EFOUT) EFOUT=1.E-8
  IF(.NOT.EFIN) EFIN=EFOUT=1.E-8
  IF(TOL.EQ.0.0) TOL=0.001
175 NOVAR = 1
  DO 157 I=1,NUMCON
    IF(NK(I))158,157
158 N1(NOVAR)=NAME(I+ISTATE)
    IF(JUMP) 8158,8159
8158 XCONST(NOVAR)=CONST(I)
8159 NOVAR=NOVAR+1
157 CONTINUE
  NODATA=0
  DO254 N=1,INDATA
    IF(WT(N))252,253
253 NUSE(N)=0
    GO TO 254
252 NUSE(N)=1
    NODATA=NODATA+1
254 CONTINUE
  NDEL=0
495 NOIN=K=NOENT=NOMIN=NOMAX=VAR=FLEVEL=0.0
  LOOP=0
  NOVMI = NOVAR - 1
  NOVPL = NOVAR + 1
  DO 176 I = 1,NOVPL
    DO 176 J = 1,NOVPL
176 VECTOR(I,J) = 0.0
    IF(NDEL)501,500
500 SUMWHT=0.0
    DO525N=1,INDATA
      NUM=0
      DO 512 I=1,NUMCON
        IF(NK(I))511,512
511 NUM=NUM+1
        DATA(NUM,N)=CON (I,N)
512 CONTINUE
        DATA(NOVAR,N)=FOBS(N)-FCALC(N)

```



```

525 SUMWHT=SUMWHT+WT(N)
501 AVEWHT=SUMWHT/NOCDATA
   DO510N=1,INDATA
   IF(NUSE(N))146,510
146 WHT=WT(N)/AVEWHT
   DO 540 I = 1, NOVAR
   VECTOR(I,NOVPL)=VECTOR(I,NOVPL)+DATA(I,N)*WHT
   DO 540 J = 1,NOVAR
541 VECTOR(I,J)=VECTOR(I,J)+DATA(I,N)*DATA(J,N)*WHT
   VECTOR(NOVPL,NOVPL) = VECTOR(NOVPL,NOVPL) + WHT
511 CONTINUE
   IF(INFO)580,650
580 PRINT 1115
1115 FORMAT(*1SUM OF VAR*/ )
   NOMAX=NOVMI
   IF(NOVMI.GT.8) NOMAX=8
   PRINT 15, (I,I=1,NOMAX)
   PRINT 17, VECTOR(NOVAR,NOVPL),(VECTOR(I,NOVPL),I=1,NOMAX)
   IF(NOMAX.EQ.NOVMI) GO TO 581
   NOMAX=NOMAX+1
   PRINT 1116,(I,I=NOMAX,NOVMI)
   PRINT 17, (VECTOR(I,NOVPL),I=NOMAX,NOVMI)
581 CONTINUE
   NGO=0 & NOMIN=1 & NOMAX=NOVMI
   IF(NOMAX=6)599,599,601
601 NOMAX=6
   NGO=1
599 PRINT 152,(I,I=NOMIN,NOMAX)
   DO 180 J=NOMIN,NOVMI
   JJJ=J
   IF(JJJ.GT.NOMAX.AND. NGO)JJJ=NOVMAX
180 PRINT 153,J,(VECTOR(I,J),I=NOMIN,JJJ)
   PRINT 154,(VECTOR(I,NOVAR),I=NOMIN,NOMAX)
   IF(NGO=1) 603,604,602
604 NOMIN=7 & NGO=0 & NOMAX=NOVMI
   IF(NOMAX.GT.12) 1601,599
1601 NOMAX=12 & NGO=2 & GO TO 599
602 NGO=0 & NOMIN=13 & NOMAX=NOVMI & GO TO 599
603 CONTINUE
   PRINT155, VECTOR(NOVAR,NOVAR)
651 NOSTEP = -1
   ASSIGN 1320 TO NUMRER
   DEFR = VECTOR(NOVPL,NOVPL) - 1.0
   DO 800 I = 1,NOVAR
   IF(VECTOR(I,I)) 792,794,810
792 PRINT 793, I
   GOT0172
794 PRINT 795, I
   SIGMA(I) = 1.0
   GO TO 800
810 SIGMA(I) =DSQRT (VECTOR (I,I))
800 VECTOR(I,I) = 1.0
   DO 830 I = 1,NOVMI
   IP1 = I + 1

```




```

      DO 830 J = IP1, NOVAR
      VECTOR(I,J) = VECTOR(I,J) / ( SIGMA(I)* SIGMA(J))
830  VECTOR(J,I) = VECTOR(I,J)
      IF(INFO)870,1001
870  PRINT159,(I,I=1,NOVM1)
      DO 885 I=2,NOVM1
      IM1=I-1
885  PRINT160,I,(VECTOR(I,J),J=1,IM1)
      PRINT161,(VECTOR(I,NOVAR),I=1,NOVM1)
1001  NOSTEP = NOSTEP + 1
      IF (VECTOR( NOVAR,NOVAR)) 1002,1002,1010
1002  NSTPM1 = NOSTEP - 1
      PRINT 1004, NSTPM1
      GO TO 1381
1010  SIGY = SIGMA(NOVAR) *DSQRT (VECTOR(NOVAR,NOVAR)/ DEFR)
      DEFR =DEFR-1.0
      IF (DEFR ) 1017,1017, 1020
1017  PRINT 1019 ,NOSTEP
      GO TO 1381
1020  VMIN=VMAX=NOIN=0
      DO 1050 I = 1,NOVM1
      IF (VECTOR(I,I)) 1042, 1050, 1060
1042  PRINT 1044, I, NOSTEP
      GO TO 1381
1060  IF(VECTOR(I,I)-TOL) 1050, 1080, 1080
1080  VAR=VECTOR(I,NOVAR)*VECTOR(NOVAR,I)/VECTOR(I,I)
      IF(VAR)1100, 1050, 1110
1100  NOIN = NOIN + 1
      INDEX(NOIN) = I
      COFN(NOIN) = VECTOR(I,NOVAR) + SIGMA(NOVAR) / SIGMA (I)
      SIGMCO(NOIN) = (SIGY / SIGMA(I)) *DSQRT (VECTOR(I,I))
      IF (VMIN) 1160,1170,904
904  PRINT 906
      GOTO172
1170  VMIN = VAR
      NOMIN = I
      GO TO 1050
1160  IF(VAR - VMIN)1050,1050,1170
1110  IF (VAR - VMAX)1050,1050,1210
1210  VMAX = VAR
      NOMAX = I
1050  CONTINUE
      IF (NOIN) 903,1240,1300
903  PRINT 907
      GO TO 172
1240  STDY=SIGY
      GO TO 1350
1300  IF(INFO)1310,1320
1310  IF (NOENT) 1311,1311,1313
1311  PRINT168, NOSTEP, K
      GO TO 1314
1313  PRINT169, NOSTEP, K
1314  IF(LOOP) FLEVEL=FL
      PRINT 162,K,FLEVEL,SIGY

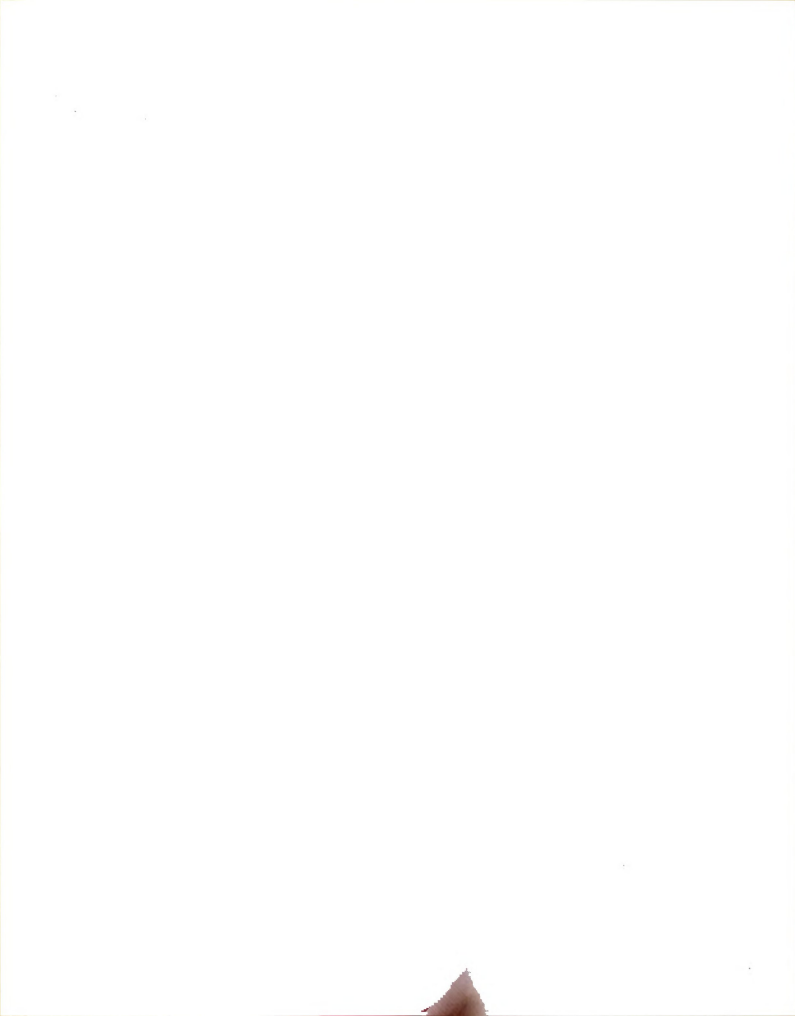
```



```

      DO1301 J=1,NOIN
      N=INDEX(J)
1301 PRINT163,N,N1(N),COEN(J),SIGMCO(J)
      IF(JUMP) 8302,8304
1302 IF(LOOP) 8303,8304
1303 PRINT 8305
1305 FORMAT(*2FINAL CONSTANTS AFTER CORRECTIONS WERE ADDED*)
      DO 8306 J=1,NOIN
      N=INDEX(J)
      XNEWCON=COEN(J)*XCONST(N)
1306 PRINT 163,N,N1(N),XNEWCON,SIGMCO(J)
1304 GO TO NUMBER,(1320,1580)
1320 FL=FLEVEL
      FLEVEL=VMIN*DEFR/VECTOR(NOVAR,NOVAR)
      IF(EFOUT + FLEVEL) 1350,1350,1340
1340 K = NOMIN
1345 NOENT = 0
      GO TO 1391
1350 FLEVEL = VMAX + DEFR / (VECTOR(NOVAR,NOVAR)- VMAX)
      IF (EFIN - FLEVEL) 1370,1361,1360
1361 IF (EFIN) 1380,1380,1370
1370 K = NOMAX
      NOENT = K
1391 IF(K) 1392,1392,1400
1392 PRINT 1395, NOSTEP
      GOT0172
1400 DO 1410 I = 1,NOVAR
      IF (I-K) 1430,1410,1430
1430 DO 1440 J = 1, NOVAR
      IF (J-K) 1460,1440,1460
1460 VECTOR(I,J)=VECTOR(I,J)-VECTOR(I,K)*VECTOR(K,J)/VECTOR(K,K)
1440 CONTINUE
1410 CONTINUE
      DO 1480 I = 1, NOVAR
      IF (I-K) 1500,1480,1500
1500 VECTOR (I,K) = - VECTOR (I,K) / VECTOR (K,K)
1480 CONTINUE
      DO 1520 J = 1, NOVAR
      IF (J-K) 1540,1520,1540
1540 VECTOR(K,J) = VECTOR (K,J) / VECTOR (K,K)
1520 CONTINUE
      VECTOR(K,K) = 1.0 / VECTOR(K,K)
      GOT0101
1380 CALL HEAD1
1381 CONTINUE
1570 ASSIGN 1580 TO NUMBER
      LOOP=1
      GO TO 1310
1580 CONTINUE
      IF(INFO) PRINT1586,(L,VECTOR(L,L),L=1,NOVM1)
      CALL HEAD2
      VFIT=DEVMAX=SWT=XIR=0.0
      DO1600 N=1,INDATA
      WTN=NUSE(N)*WT(N)

```



```

      WHT=WTN/AVEWHT
      YPRED = 0.0
      DO 1630 I = 1,NOIN
1630  YPRED=YPRED+COEN(I)*DATA(INDEX(I),N)
      DEV=FOR(N)-FCALC(N)=YPRED
      IF(10.-WT(N))1652,1652,1651
1651  VFIT=VFIT+WTN*DEV**2
      XIR=XIR+1.0
      SWT=SWT+WT(N)
1652  FREOPRD=FCALC(N)+YPRED
      WHT=WHT*AVEWHT
      CALL OUTPUT
      ADEV=ARSF(DEV)*SQRTF(WHT)*NUSE(N)
      IF(DEVMAX-ADEV)1610,1610,1660
1610  NMAX=N
      DEVMAX=ADEV
1660  CONTINUE
      VFIT=VFIT*XIR/((XIR-NOIN)*SWT)
      STDFIT=SQRTF(VFIT)
      PRINT150, VFIT, STDFIT
      IF(NDELMAX=NDEL)172,172,1624
1624  IF(DEVMAX-XDEVMAX)172,172,1620
1620  NUSE(NMAX)=0
      NDEL=NDEL+1
      NODATA=NODATA-1
      SUMWHT=SUMWHT-WT(NMAX)
      PRINT 9001,NMAX
      GOTO495
172  RETURN
      15  FORMAT(*          Y*8I15,/)
      17  FORMAT(* *9F15.4,/)
1116  FORMAT(17,8I15,/)
123  FORMAT (I11,A9* NO CORRECTION FOUND*)
150  FORMAT(*0STAT FROM LINES WHTD LT 10.0*/*0VAR. **F10.6*      STD. DE
      1V **F7.4/*7*)
151  FORMAT (10A8)
152  FORMAT(*-RAW SSCP MATRIX*/121,5I22)
153  FORMAT(X12,6F22.4)
154  FORMAT(*   Y*6F22.4)
155  FORMAT(*   Y VS Y*F15.4)
156  FORMAT (13I1,35X12,10X15,F5,2XA8)
159  FORMAT (*-PARTIAL CORR. COEFF.*//16I8)
160  FORMAT (13,16F8.4)
161  FORMAT (*   Y*16F8.4)
162  FORMAT (*   F LEVEL OF X-*I1,E10.2,9X*STD DEV OF (O-P)*F7.4//10X*V
      1ARIABLE      COEFFICIENT      STD ERROR*/)
163  FORMAT (I11,A9,2F17.12)
168  FORMAT (*0STEP NO*13/*      VAR. REMOVED*13)
169  FORMAT (*0STEP NO*13/*      VAR. ENTERED*13)
171  FORMAT(*2RESULTS*//*      COEFFICIENT      OLD VALUE      CORRECT
      1ION      NEW VALUE*//8(9XA6,3F15.8/),4(9XA6,4X3F15.12/))
701  FORMAT (4F15)
702  FORMAT (*ABOVE NCN=EIGENVALUE NOT DIAG. AFTER 10 CYCLES*)
793  FORMAT (* ERROR RESID SQ VAR*13* IS NEG*)

```



```

795 FORMAT (*QVAR*I5* IS CONST*)
850 FORMAT (X6I3,F20,F10,23XA8)
904 FORMAT (*QERROR, VMIN POS*)
907 FORMAT (*QERROR NOIN NEG*)
1000 FORMAT (*QLINE NO*I4* DELETED*5X6I3,2F10.4)
1004 FORMAT (*QY SQUARE NEG STEP*I5)
1019 FORMAT (*QZERO DEG FREEDOM STEP*I3)
1044 FORMAT (*SQUARE X-*I2* NEGATIVE STEP*I3)
1395 FORMAT (*K=0 STEP*I3)
1586 FORMAT (*Q DIAG ELEMENTS*/ * VAR NO      VALUE*//(I4,F12.6))
9000 FORMAT (2I5,F10)
9001 FORMAT (*+LINE NO*I4* BEING DELETED FROM FIT*)
      END

```

```

SUBROUTINE PRINTOUT
COMMON/1/NOADATA,NOVMI,AVEWHT,STDY,NOSTEP,N,WTN,FREQPRD,YPRED,DEV,
1DATA(20,500)
COMMON/2/FOBS(500),FCALC(500),WT(500),NK(17),INFO,INDATA,NDELMAX,
1XDEVMAX,N1(25),MOL,CON(17,500),IH(10),SS(500),VV(500),KK(500),
2JJ(500),NUMCON,ISTATE
COMMON/3/ NOVAR,JUMP,CONST(20),EFIN,EFOUT
COMMON/5/ TOL
COMMON/10/ IFUNCH
COMMON/C/ NAME(30)
TYPE INTEGER SS,VV,BRANCH
ENTRY ROTCONS1
PRINT 167,MOL,NOADATA,NOVMI,NDELMAX,XDEVMAX,AVEWHT,STDY,NOSTEP
RETURN
ENTRY ROTCONS2
PRINT166
RETURN
ENTRY ROTCONS3
PRINT 165, N,SS(N),VV(N),KK(N),JJ(N),WTN,FOBS(N),FCALC(N),FREQPRD,
1DATA(NOVAR,N),YPRED,DEV
IF(IFUNCH) PUNCH 1165,N,SS(N),VV(N),KK(N),JJ(N),WTN,FOBS(N),
1FREQPRD,DEV
RETURN
ENTRY SPORCON1
PRINT 267, MOL,NOADATA,NOVMI,NDELMAX,XDEVMAX,AVEWHT,STDY,NOSTEP
RETURN
ENTRY SPORCON2
PRINT 266
RETURN
ENTRY SPORCON3
PRINT 265, N,VV(N),JJ(N),WTN,FOBS(N),FCALC(N),FREQPRD,DATA(NOVAR,N
1),YPRED,DEV
RETURN
ENTRY FREQFIT1
PRINT 367,MOL,NOADATA,NOVMI,NDELMAX,XDEVMAX,AVEWHT,STDY,NOSTEP
RETURN
ENTRY FREQFIT2
PRINT 366
RETURN
ENTRY FREQFIT3

```




```

      BRANCH=KK(N)+50
      PRINT 465,N,VV(N),BRANCH,SS(N),JJ(N),WTN,FOBS(N),FCALC(N),FREQPRD,
1 DATA(NOVAR,N),YPRED,DEV
      RETURN
      ENTRY FITALL1
      PRINT 367,MOL,NODATA,NOVMI,NDELMAX,XDEVMAX,AVEWHT,STDY,NOSTEP
      RETURN
      ENTRY FITALL2
      PRINT 466
      RETURN
      ENTRY FITALL3
      IF(SS(N).EQ.3) SS(N)=1RH
      IF(SS(N).EQ.4) SS(N)=1RL
      BRANCH=KK(N)+1RQ
      PRINT 465,N,VV(N),BRANCH,SS(N),JJ(N),WTN,FOBS(N),FCALC(N),FREQPRD,
1 DATA(NOVAR,N),YPRED,DEV
      IF(IPUNCH) PUNCH 1465,N,VV(N),BRANCH,SS(N),JJ(N),WTN,FOBS(N),
1 FREQPRD,DEV
      RETURN
      ENTRY LAMCON1
      PRINT 567,MOL,NODATA,NOVMI,NDELMAX,XDEVMAX,AVEWHT,STDY,NOSTEP
      RETURN
      ENTRY LAMCON2
      PRINT 566
      RETURN
      ENTRY LAMCON3
      PRINT 565,N,SS(N),KK(N),JJ(N),WTN,FOBS(N),FCALC(N),FREQPRD,
1 DATA(NOVAR,N),YPRED,DEV
      IF(IPUNCH) PUNCH 1565,N,SS(N),KK(N),JJ(N),WTN,FOBS(N),FREQPRD,DEV
      RETURN
165 FORMAT (15,3I2,I3,*/2*,F6.2,6F9.4)
166 FORMAT (*1 NO S V K J WHT OBS CALC PRED O-C
1 P-C O-P*)
167 FORMAT (*1 COMBINATION DIFFERENCES FOR *A8/* FIT *I4* DATA POINTS
1 TO * I2* VARIABLES*/* DELETES UP TO *I2* POINTS IF (O-P) IS
2 GT *F6.3/* WHT NORM *F6.2/* STD DEV OF (O-C) * F9.4/* CO
3 MPLETED *I2* STEPS*)
265 FORMAT (15,I4,I5,*/2*,F6.2,6F9.4)
266 FORMAT (*1 NO V J WHT OBS CALC PRED O-C
1 P-C O-P*)
267 FORMAT (*1 SPIN ORBIT DIFFERENCES FOR *A8/* FIT *I4* DATA POINTS I
1 0 * I2* VARIABLES*/* DELETES UP TO *I2* POINTS IF (O-+) IS GT
2 *F6.3/* WHT NORM *F6.2/* STD DEV OF (O-C) * F9.4/* COMPL
3 ETED *I2* STEPS*)
366 FORMAT (*1 NO V LINE WHT OBS CALC PRED O-C
1 P-C O-P*)
367 FORMAT (*1 FREQUENCY FIT FOR *A8/* FIT *I4* DATA POINTS TO *I2* VA
1 RIABLES*/* DELETES UP TO *I2* POINTS IF (O-P) IS GT *F6.3/*
2 WHT NORM *F6.2/* STD DEV OF (O-C) *F9.4/* COMPLETED *I2*
3 STEPS*)
465 FORMAT(X,I3,I2,1X,2R1,I3,*/2*1X,F4.2,3F11.4,3F9.4)
466 FORMAT(*1 NO V LINE WHT OBS CALC PRED O-C
1 P-C O-P*)
565 FORMAT(X,I3,X,2R1,I3,*/2 *F4.2,X,2F8.4,4F9.4)

```



```

566 FORMAT(*1 NO LINE WHT OBS CALC PRED O-C
      1P-C O-P*)
567 FORMAT(*1 LAMDA DIFFERENCE FIT FOR*A8/ * FIT *I4* DATA POINTS
      1TO* I2* VARIABLES*/* DELETES UP TO *I2 * POINTS IF (O-P) IS
      2 GT*F6.3/* WHT NORM*F6.2/* STD DEV OF (O-C)* F9.4/* CO
      3MPLETED *I2* STEPS*)
1165 FORMAT(I5,3I2,I3,*/2*,F6.2,3X,3F15.4)
1465 FORMAT(I5,I3,X,2R1,I3,*/2*,F6.2,3X,3F15.4)
1565 FORMAT(I5,2X,2R1,I3,*/2*,F8.2,3X,3F15.4)
      END

```


G. ZEEPUN

This program calculates the Zeeman splittings for all branches for the intermediate coupling case and for specified values of field strength. Punch output of these is provided for later input to the plotting program. Inputs include the spin-orbit and rotational constants for the transition under consideration, the Zeeman splitting constant, the vibration-rotation band, the fields to be used and the J-values desired. Also available is the option of adding a fixed value to all splittings.

STRUCTURE OF DATA DECK

I. Punch option card

<u>Col.</u>	<u>Field</u>	<u>Function</u>
1-9	I	≠0 indicates punch section is desired.
10,11,12	R	Beginning in col. 10; P, Q, and R indicates that punch output of these branches is desired. One or all may be used.
20-29	I	≠0 indicates punch output is desired.

II. Constants card

These three cards contain the values of the molecular constants A and B and the Zeeman splitting constant respectively. The cards are read from left to right and have 8 fields of 10 columns. The constants A and B are punched on the first two cards in the order $v = 0, 1, 2, 3$ for $^{14}\text{N}^{16}\text{O}$ and $^{15}\text{N}^{16}\text{O}$ respectively. The Zeeman constant is on the third card in cols. 1-10.



III. Band card

The band designation is typed in cols. 1-10 of this card. The codes are: (1-0) = 1, (2-0) = 2, (3-0) = 3, HES = 4, LES = 5. The format is I10.

IV. Field strength card

Up to 8 values of field may be input and the splitting is automatically calculated for each. The value is input in gauss; there are 8 fields of 10 columns starting from the left of the card. The format is 8(F10.1).

V. J-value card

This card specifies the J-value(s) desired and provides for adding a constant value to the splittings. The option of choosing only one subband is also available. As many of these cards as needed may appear.

<u>Col.</u>	<u>Field</u>	<u>Function</u>
12-13	I	2J
20-32	F	≠0 indicates that this value should be added to all splittings.
41-50	I	A value of 1 or 2 will indicate that only that subband is desired. A blank will cause calculation for both.
73-80	A	If the word COMPLETE appears, splittings of all transitions up to and including J are calculated.

VI. Return card

If RETURN appears in cols. 75-80, control is returned to I.

VII. New case card

If NEW CASE appears in cols. 73-80, control is returned to

section III.

VIII. Stop card

If STOP appears in cols. 77-80, execution is terminated.

A listing of the program follows.


```

PROGRAM ZEEPUN
COMMON/1/ FREQ(300),XINT(300)
COMMON/4/ IJIM, IBRANCH(3),IPUNCH
100 READ 1, IJIM, (IBRANCH(N),N=1,3),IPUNCH
1  FORMAT (19,3R1,7X,I10)
   DO 3 L=1,3
3  IBRANCH(L)=IBRANCH(L)-1R0
   CALL ZEEMAN
   GO TO 100
END
SUBROUTINE ZEEMAN
COMMON/1/ FREQ(300),XINT(300)
COMMON/4/ IJIM, IBRANCH(3),IPUNCH
DIMENSION DA(10),A(5,10),DR(10),B(5,10),DG(100,2,1),G(100,2,5),
1      H(10),Y(3)
DIMENSION ISIGN(2),FRQ(50,2,3),INT(50,2,3)
DATA(ISIGN=1,-1)
TYPE REAL INT
N=0
READ 1,((A(I,J),J=N,3),I=1,2),((B(I,J),J=N,3),I=1,2),AMU0
1  FORMAT (8F10,5,/,8F10,5,/,F10)
2  READ 3, IMOL
3  FORMAT (10X,I2)
   READ 1001, IBAND
1001 FORMAT (I10)
   READ 1002, (H(I),I=1,8)
1002 FORMAT (8F10,1)
9999 READ 1003, JMAX,XNU,ISUBAND,IPLT
1003 FORMAT (11X,I2,6X,F13.4,8X,I10,22X,A8)
   IF(IPLT.EQ.8H STOP) GO TO 5000
   IF(IPLT.EQ.8HNEW CASE) GO TO 2
   IF(IPLT.EQ.8H RETURN) RETURN
   H(9)=0.0
   JMOL=IMOL-13
4  CONTINUE
   LMAX=(JMAX+1)/2
   JF=8
   DO 61 J=1,JF
   IF(H(J+1).EQ.0.0)JF=J
   FLDFAC=AMU0*H(J)
   FIELD=H(J)
   FU=FL=-1.0
   GO TO (5,6,7,8,9),IBAND
5  NJ=2
   NU=NL=KU=1
   KL=0
   EPSU=EPSL=-1.0
   GO TO 15
6  NJ=2
   NU=NL=1
   KU=2
   KL=0
   EPSU=EPSL=-1.0
   GO TO 15

```

```

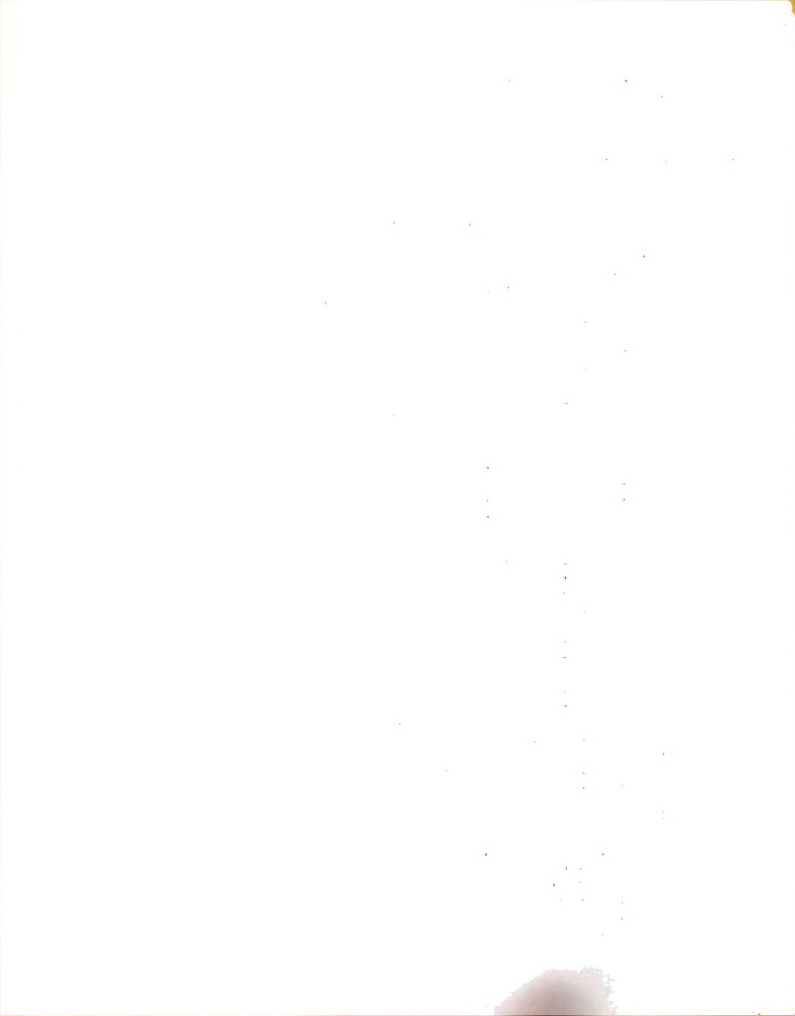
7  NJ=2
   NU=NL=1
   KU=3
   KL=0
   EPSU=EPSL=-1.0
   GO TO 15
8  NJ=NL=KU=ITRL=1
   NU=2
   KL=0
   EPSU=1.0
   EPSL=-1.0
   ITRU=3
   GO TO 15
9  NJ=NU=KU=ITRU=1
   NL=2
   KL=0
   EPSU=-1.0
   EPSL=1.0
   ITRL=3
15 CONTINUE
   Y(KU)=A(JMOL,KU)/B(JMOL,KU)
   Y(KL)=A(JMOL,KL)/B(JMOL,KL)
   IF(ISUBAND) 9100,9200
9100 NB=NT=ISUBAND
   IF(ISUBAND,EQ.2) FU=FL=1.0
   GO TO 9000
9200 NB=1
   NT=NJ
9000 DO 61 M=NB,NT
   IF(M,EQ.2) NU=NU+1
   IF(M,EQ.2) NL=NL+1
   FU=FU*EPSU
   FL=FL*EPSL
   JJ=LMAX+1
   IGO=1
   DO 20 L=1,JJ
   IF(IPLT,NE,8HCOMPLETE) 202,201
202 IF(IGO) 200,201
200 L=LMAX+1
   IGO = 0
201 AQ=L*.5
   AM=AQ*(AQ+1.0)
   G(L,NU,KU)=(1.5+FU*((2.0*(AM*.75))-1.5*Y(KU)+3.0)/SQRT(4.0*AM+1.0+
1Y(KU)*(Y(KU)-4.0)))/AM
   G(L,NL,KL)=(1.5+FL*((2.0*(AM*.75))-1.5*Y(KL)+3.0)/SQRT(4.0*AM+1.0+
1Y(KL)*(Y(KL)-4.0)))/AM
20 CONTINUE
   DO 61 L=1,LMAX
   IF(IPLT,NE,8HCOMPLETE) 300,301
300 L=LMAX
301 ASSIGN 51 TO NGOTO
   AQ=L*.5
   JQ=2*L+1
   IF(NL,EQ,2.AND,L.LT,2)GO TO 60

```

```

      IF(NU.EQ.NL) 2000,2100
2000  ISUB=NU
      PRINT 31, IMOL,KU,NU,JQ,H(J)
      GO TO 50
2100  IF(NU.NE.NL) 2200,50
2200  IF(ITRU=ITRL) 2300,2300,2400
2300  ISUB=1RL
      GO TO 2500
2400  ISUB=1RH
2500  PRINT 41, IMOL,KU,ITRL,ITRU,JQ,H(J)
50    JM=L+L
      I=2*JM
      SUMP=1.333*AQ*(2.*AQ+1.)*(2.*AQ-1.)
      SUMQ=1.333*AQ*(AQ+1.)*(2.*AQ+1.)
      SUMR=1.333*(AQ+1.)*(2.*AQ+1.)*(2.*AQ+3.)
      DO 60 K=1,JM
      LJ=L+K
      AJ=LJ-.5
      ALPHA=G(L,NL,KL)*FLDFAC*AJ
      ZETAR=(AJ-1.0)*FLDFAC
      ZETAL=(AJ+1.0)*FLDFAC
      DNUPL=DNUPR=DNUQL=DNUQR=DNURL=DNURR=RITNPL=RITNPR=RITNQL=RITNQR=
1    RITNRL=RITNRR=10**10
      IF(L,GE.3) GO TO NGOTO
      IF(NU.EQ.2.AND.L,LT.3) ASSIGN 52 TO NGOTO
      IF(NU.EQ.1.AND.L,LT.2) ASSIGN 52 TO NGOTO
      IF(NU.EQ.2.AND.L,LT.2) ASSIGN 53 TO NGOTO
      IF(NL,EQ.2.AND.L,LT.2) ASSIGN 53 TO NGOTO
      GO TO NGOTO
51    DNUPR=G(L+1,NU,KU)*ZETAR=ALPHA
      DNUPL=G(L+1,NU,KU)*ZETAL=ALPHA
      RITNPR=((AQ-AJ)*(AQ-AJ+1.0))*100./SUMP
      RITNPL=((AQ-AJ)*(AQ-AJ+1.0))*100./SUMP
52    DNUQR=G(L,NU,KU)*ZETAR=ALPHA
      DNUQL=G(L,NU,KU)*ZETAL=ALPHA
      RITNQR=((AQ-AJ)*(AQ-AJ+1.0))*100./SUMQ
      RITNQL=((AQ-AJ)*(AQ-AJ+1.0))*100./SUMQ
53    DNURR=G(L+1,NU,KU)*ZETAR=ALPHA
      DNURL=G(L+1,NU,KU)*ZETAL=ALPHA
      RITNRR=((AQ-AJ+1.0)*(AQ-AJ+2.0))*100./SUMR
      RITNRL=((AQ-AJ+1.0)*(AQ-AJ+2.0))*100./SUMR
      IF(RITNPL,EQ,0.0)DNUPL=RITNPL=10**10
      IF(RITNPR,EQ,0.0)DNUPR=RITNPR=10**10
      IF(RITNQL,EQ,0.0)DNUQL=RITNQL=10**10
      IF(RITNQR,EQ,0.0)DNUQR=RITNQR=10**10
      IF(RITNRL,EQ,0.0)DNURL=RITNRL=10**10
      IF(RITNRR,EQ,0.0)DNURR=RITNRR=10**10
      INDEX=2*LJ=1
      PRINT55,INDEX,DNUPL,RITNPL,DNUPR,RITNPR,DNUQL,RITNQL,DNUQR,RITNQR,
1    DNURL,RITNRL,DNURR,RITNRR
      IF(IJIM) 500,60
500   FRQ(K,1,1)=DNUPL*XNU
      INT(K,1,1)=RITNPL
      FRQ(K,2,1)=DNUPR*XNU

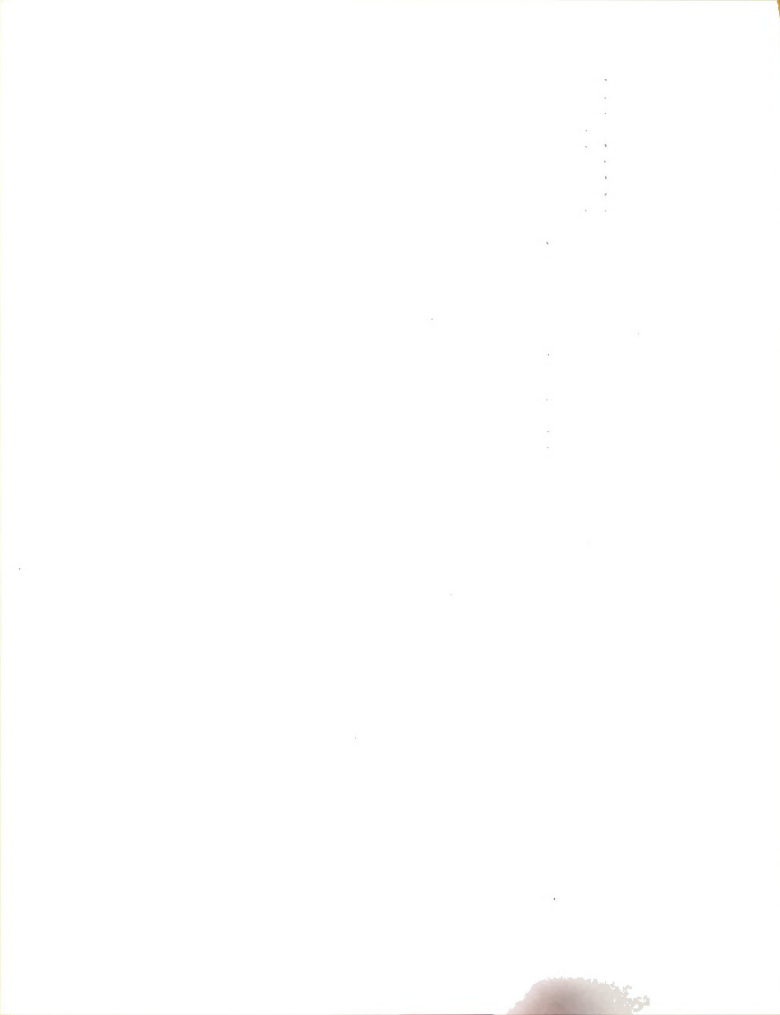
```



```

      INT(K,2,1)=RITNPR
      FRQ(K,1,2)=DNUQL+XNU
      INT(K,1,2)=RITNQL
      FRQ(K,2,2)=DNUQR+XNU
      INT(K,2,2)=RITNQR
      FRQ(K,1,3)=DNURL+XNU
      INT(K,1,3)=RITNRL
      FRQ(K,2,3)=DNURR+XNU
      INT(K,2,3)=RITNRR
60  CONTINUE
      IF(IJIM)801,61
801  DO 900 LI=1,3
      IF(IBRANCH(LI).GT.5) GO TO 61
      NAME=IBRANCH(LI)+1R0
      IF(IPUNCH) PUNCH 5500, NAME, ISUB,JQ,IMOL,FIELD
5500 FORMAT(10X,2R1,X,I2,*/2*,2X,*N*I2*0*,6X,F10,1,*GAUSS*)
      DO 800 KI=1,JM
      DO 800 JI=1,2
      IF(FRQ(KI,JI,IBRANCH(LI)).GT.5000) 799,850
850  FREQ(KI+(JI-1)*JM)=FRQ(KI,JI,IBRANCH(LI))
      XINT(KI+(JI-1)*JM)=INT(KI,JI,IBRANCH(LI))*ISIGN(JI)
      GO TO 800
799  FREQ(KI+(JI-1)*JM)=0,0
      XINT(KI+(JI-1)*JM)=0,0
800  CONTINUE
      NUM=0
      DO 3000 N=1,I
      IF(.NOT.FREQ(N)) GO TO 3000
      NUM=NUM+1
      FREQ(NUM)=FREQ(N)
      XINT(NUM)=XINT(N)/100.
3000 CONTINUE
      IF(IPUNCH) PUNCH 5501,(FREQ(KQ),XINT(KQ),KQ=1,NUM)
5501 FORMAT (4(2(F7.4,3X)))
900  CONTINUE
61  CONTINUE
      GO TO 9999
5000 CONTINUE
55  FORMAT(I4*/2*3(2(2XF7.4,XF3)X))
31  FORMAT(*1  CALCULATION OF ZEEMAN SPLITTINGS AND RELATIVE INTENSIT
11ES FOR,*/*  N*I2*0, *I1*-0, BAND, *I1*-SUBBAND.*/*  J = *I2*
2/2, H =*F5* GAUSS.*/*--18X*P BRANCH*17X*Q BRANCH*17X*R
3 BRANCH*/*0 MJ*3(* DELM+ I DELM- I*X)/)
41  FORMAT(*1  CALCULATION OF ZEEMAN SPLITTINGS AND RELATIVE INTENSIT
11ES FOR,*/*  N*I2*0, *I1*-0, *I1*/2 - *I1*/2 BAND.*/*  J = *I
22*/2, H =*F5* GAUSS.*/*--18X*P BRANCH*17X*Q BRANCH*17X
3*R BRANCH*/*0 MJ*3(* DELM+ I DELM- I*X)/)
      END

```

H. PLOTPUN

This program accepts input of intensities and splittings symmetric about the origin, and calculates and plots the absorption, Zeeman and magnetic rotation signals expected. Gaussian and intermediate lineshapes are available; Gaussian, triangular and trapezoidal slit-functions are available. The Doppler, Lorentz and slit-function HWHM, pressure, polarizer angle and path lengths are input.

STRUCTURE OF DATA DECK

I. Option card

<u>Col.</u>	<u>Field</u>	<u>Function</u>
1	I	= 1, 2, or 3; indicates that a Gaussian, triangular or trapezoidal slit-function is desired.
2	I	≠0; calculates rotation angle per unit path length.
3	I	≠0; calculates the individual transmission fractions for all components. =2; plots the unintegrated CD pattern.
4	I	≠0 calculates the unintegrated circular birefringence. =2, plots the unintegrated CB pattern.
5	I	≠0; plots the transmission fraction for right and left circular polarizations.
6	I	≠0; calculates the CD pattern integrated over the slit-function. =2; plots the above.
7	I	≠0; calculates the CB integrated over the slit-function. =2; plots the above.



<u>Col.</u>	<u>Field</u>	<u>Function</u>
8	I	≠0; plots the integrated MR signal.
9	I	≠0; plots the unintegrated MR signal.
10	I	plots a title according to the code; 1-CIR. DICHOISM, 2-TRANSMISSION, 3-ABS. COEFFICIENT, 4-MAG. ROTATION, 5-ZEEMAN, 6- ABSORPTION, 7-blank.
11	I	≠0; causes all plots above to be superimposed.
12	I	≠0; plots the integrated absorption.
13	I	≠0; prints values of all quantities. =1; every 5th plotter unit printed. =2; every plotter unit printed. =3; every 2nd plotter unit printed. =4; every 10th plotter unit printed.
14	I	≠0; suppresses the plot of the experimental conditions.
15	I	≠0; plots bar graph of the Zeeman patterns.
21-30	F	Doppler HWHM.
31-40	F	Lorentz HWHM, an intermediate (Doppler) lineshape is used if this is non-zero (zero).
41-50	F	Range in $\text{cm}^{-1}/10''$ of the plot.
51-60	F	Height of the plot in intensity units/inch.
61-70	F	Slit-function HWHM.
71-75	F	≠0; uses trapezoidal slit-function. This is the halfwidth of the top of the trapezoid.
76-80	F	A tolerance used to control the intervals of integration in calculating the lineshape. The intervals are normally 0.001 times the range in cols. 41-50 above. The tolerance may be set to some fraction of this value. It is preset to 1.0.

II. Pressure card

Values of the pressure are read by the format 8F10. The calculations specified on the option card are automatically repeated for every pressure.

III. Any of the following cards may appear

1. Absorption card: The integrated absorption coefficient for the transition is input in cols. 1-10, the path length in cm. is in cols. 11-20 and the polarizer angle in degrees is in cols. 21-30. The splittings and relative intensities follow this card.
2. New case card: If NEW CASE is encountered in cols. 73-80, control is returned to section I.
- 3) Stop card: If STOP is encountered in cols. 77-80 execution is terminated.

IV. Splitting cards

These cards follow card III-1 above. The splittings and intensities must be symmetric about the origin as input.

1. Title card: This card is the title card punched in ZEEPUN. It specifies the transition and field strength.
2. Splitting cards: The splittings and fractional intensities from ZEEPUN are input here.
3. Blank card: A blank card signifies the end of input data.

V. Control card

Upon completion of all options for the last pressure, control is returned to section III.

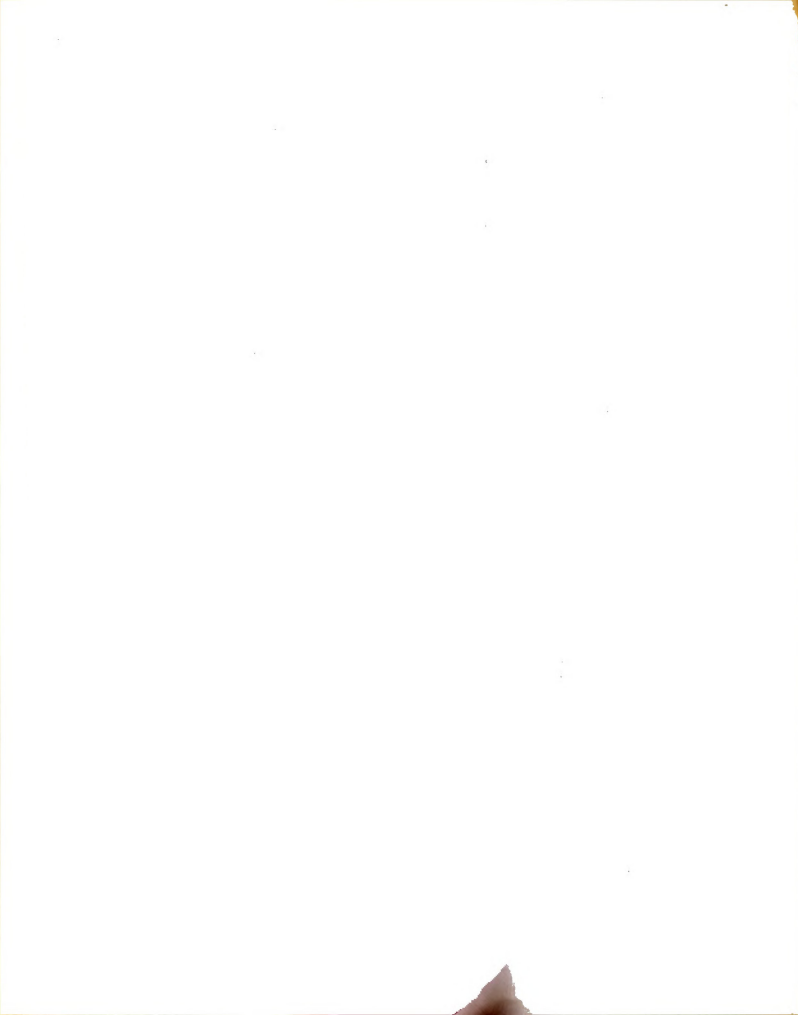
A listing of the program follows.



```

PROGRAM PLOTPUN
COMMON/1/ XNU(300),A(300)
COMMON/2/ DABSCOFM(601),ABSCOFM(600),DABSCOFF(601),ABSCOFF(600)
COMMON/3/ SY,SX,MAXPOS,GAML,GAMD, IOP(20),NUMBER,XMAX,NUMM
COMMON/4/ DSHAPE(601),SHAPE(600),IMAX,IMIN,SLITWIDTH,POL,SLITTRAP
COMMON/5/ ILABEL(4),FIELD
COMMON/6/ RANGE,HEIGHT,S0,P(8),PRES,OPL,XNUZERO,SLITNORM,TOL
COMMON/7/ DTRANSP(601),TRANSP(600),DTRANSP(601),TRANSP(600),
1DCD(601),CD(600)
COMMON/8/ DPHI(601),PHI(600)
COMMON/9/ DFARADAY(601),FARADAY(600)
COMMON/10/ DCDINT(601),CDINT(600),DFARINT(601),FARINT(600)
COMMON/11/ DLNSHP(601),XLNSHP(600)
DIMENSION LABEL(4)
DIMENSION I1(4),I2(4)
DIMENSION NAME1(10),NAME2(10)
DATA(I1=1,-1,1,-1),(I2=0,1,0,1)
DATA(NAME1=8HCIR, DIC,8HTRANSNIS,8HABS. COE,8HMAG. ROT,8HZEEMAN ,
18HABSORPTI,8H      ),(NAME2=8HHROISM ,8HSION ,8HEFFICIENT,8HA
2TION ,8H      ,8HON ,8H      )
NUMBER=0
95 READ 90, IOP,GAMD,GAML,RANGE,HEIGHT,SLITWIDTH,SLITTRAP,TOL
97 FORMAT (20I1,5F10,2F5)
IF(IOP(15)) IOP(14)=1
IF(.NOT.TOL) TOL=1.0
PLHT=6.
IF(HEIGHT) PLHT=HEIGHT/100.
KALL=1
PTEST=.
IF(.NOT.IOP(10)) IOP(10)=1
READ 91,P
91 FORMAT(8F10)
99 READ 2,S0,OPL,POLANGLE,XNUZERO,ITEST
2 FORMAT (3F10,19X,F10,13X,A8)
IF(.NOT.POLANGLE) POLANGLE=0.
POL=POLANGLE/57.29578
IF(ITEST.EQ.8HNEW CASE) GO TO 95
IF(ITEST.EQ.8H STOP) GO TO 80
READ 92, ILABEL,FIELD
92 FORMAT(10X,2R1,X,I2,5X,I2,7X,F10)
81 N=1 & NM=4
82 READ 83, (XNU(J),A(J),J=N,NM)
83 FORMAT (4(2F10))
DO 87 J=N,NM
IF(XNU(J)) GO TO 85
87 CONTINUE
86 N=N-1
IF(XNU(N)) 88,86
85 N=N+4
NM=N+3
GO TO 82
88 IFREQ=N
DO 4 J=1,IFREQ
L=J+1

```

```

DO 4 K=L,IFREQ
  IF(XNU(J).LE.XNU(K))4,3
3 T=XNU(J)  $ S=A(J)
  XNU(J)=XNU(K)  $ A(J)=A(K)
  XNU(K)=T  $ A(K)=S
4 CONTINUE
PRINT 200,ILABEL,FIELD
PRINT 202
PRINT 201, (XNU(J),A(J),J=1,IFREQ)
NN=1
1 PRES=P(NN)
  NN=NN+1
  IF(.NOT.GAML) GO TO 11
  IF(PTEST-PRES) KALL=1
  PTEST=PRES
11 CONTINUE
PRINT 203, GAMD
PRINT 1203, GAML
PRINT 204, SLITWPTH
PRINT 205, SQ
PRINT 206, OPL
PRINT 207, PRES
PRINT 208, POLANGLE
IM=-600
DO 7 IN=IM,600
  ABSCOFM(IN)=0. $ ARSCOFM(IN)=0.
  TRANSM(IN)=1.0 $ TRANSP(IN)=1.0 $ CD(IN)=0.
  PHI(IN)=0.
  FARADAY(IN)=0. $ COINT(IN)=0. $ FARINT(IN)=0.
  XLNSHP(IN)=0.
7 CONTINUE
XMAX=0
NUMM=0
ASSIGN 150 TO NGC
9000 IF(NUMBER) GO TO 16
  CALL PLOT(-4.,31.,0,100.,100.)
  CALL PLOT(0.,0.,1)
  CALL PLOT(0.,-2.,0)
  X=0. $ Y=0. $ NUMBER=1 $ NUMBER1=1 $ JUM=1 $ GO TO 17
16 NUMBER=NUMBER+1
  NUMBER1=NUMBER/2.+1
  NUM=XMODF(NUMBER,4)+1
  JUM=XMODF(NUMBER,2)
  X=15.*I1(NUM)
  Y=10.*I2(NUM)
17 CALL PLOT(Y,X,2,100.,100.)
  CALL PLOT(0.,0.,0)
  IF(.NOT.JUM) GO TO 19
  JUB=20.*NUMBER1
  CALL PLOT(JUB,0.,3)
19 CONTINUE
  IF(IOP(15)) GO TO 21
  XPLHT=PLHT+.1
  CALL CHAR(XPLHT,1.,NAME1(IOP(10)),8,0.,.2,.2)

```



```

      CALL CHAR(XPLHT,3.,NAME2(IOP(10)),8,0...2..2)
      CALL PLOT(PLHT,10.,2)
      CALL PLOT(PLHT,0.,1)
21  CONTINUE
      CALL PLOT(0.,5.,2)
      CALL PLOT(0.,0.,0)
      IF(RANGE) GO TO 8001
      DEL=XNU(IFREG)-XNU(1)
      RANGE = DEL+DEL*.1
8000  IF((RANGE-DEL)/2..GT.6+GAMN) GO TO 8001
      RANGE=RANGE+.1+DEL
      GO TO 8000
8001  CONTINUE
      XSCALE=10./RANGE
      SX=1000./RANGE
      MAXPOS=SX
      SY=600.
      IF(HEIGHT) SY=HEIGHT
      N=0
      TICS=RANGE/20.
      DO 1000 J=N,6
      XTICS=(TICS)*10.**J
      IF(XTICS.LT.1.) GO TO 1000
      IF(XTICS.LT.1.5) GO TO 1001
      IF(XTICS.LT.2.5) GO TO 1002
      GO TO 1003
1000  CONTINUE
1001  DELX=1.*(10.**(-J))
      ID=5
      GO TO 1004
1002  DELX=2.*(10.**(-J))
      ID=5
      GO TO 1004
1003  DELX=5.*(10.**(-J))
      ID=2
1004  NUMTICS=RANGE/(2.*DELX)
      D=5./XSCALE
      CALL PLOT(0.,-D,2,100.,SX)
      MAX=NUMTICS*2
      X=(NUMTICS)*DELX
      XN=-X
      NUMBIG=NUMTICS/ID
      LL=NUMTICS-NUMBIG*ID
      CALL PLOT(0.,X,1,100.,SX)
      DO 1010 L=N,MAX
      YU=.05 $ YD=-.05
      IF(L.NE.LL) GO TO 1030
      YU=.1 $ YD=-.1 $ LL=LL+ID
1030  CALL PLOT(YU,X,1)
      CALL PLOT(YD,X,1)
      CALL PLOT(0.,X,1)
      IF(L.EQ.MAX) GO TO 1010
      X=X+DELX
      CALL PLOT(0.,X,1)

```



```

1010 CONTINUE
      CALL PLOT(0.,0.,1,100.,SX)
      X=XN-.3125/XSCALE
      ENCODE(5,2501,IX2) XN
2501  FORMAT (F5.3)
      CALL CHAR(-.2,X,IX2,5,0.,.1,.1)
      XN=-XN
      X=XN-.375/XSCALE
      ENCODE(6,2500,IX1) XN
2500  FORMAT(F6.3)
      CALL CHAR(-.2,X,IX1,6,0.,.1,.1)
      CALL PLOT (0.,0.,2)
      IF(IOP(14)) GO TO 2600
      CALL PLOT (0.,-5.,2,100.,100.)
      CALL PLOT (0.,0.,0)
      ENCODE(1,5100,LABEL(2)) ILABEL(2)
      ENCODE(1,5100,LABEL(1)) ILABEL(1)
5100  FORMAT(1R1)
      ENCODE(2,5001,LABEL(3)) ILABEL(3)
      ENCODE (2,5001,LABEL(4)) ILABEL(4)
5001  FORMAT (I2)
      CALL CHAR(-.5,1.,LABEL(1),1,0.,.1,.1)
      CALL CHAR(-.5,1.1,LABEL(2),1,0.,.1,.1)
      CALL CHAR(-.5,1.28,LABEL(3),2,0.,.1,.1)
      CALL CHAR(-.5,1.5,2H/2,2,0.,.1,.1)
      CALL CHAR(-.5,1.8,1HN,1,0.,.1,.1)
      CALL CHAR(-.5,1.9,LABEL(4),2,0.,.1,.1)
      CALL CHAR(-.5,2.2,1H0,1,0.,.1,.1)
      CALL CHAR(-.5,2.6,2HH=,2,0.,.1,.1)
      NFIELD=FIELD
      ENCODE(4,300,LF) NFIELD
300  FORMAT(I4)
      CALL CHAR(-.5,2.85,LF,4,0.,.1,.1)
      CALL CHAR(-.5,3.45,5HGAUSS,5,0.,.1,.1)
      ENCODE(4,2502,LPRES) PRES
2502  FORMAT(F4.1)
      CALL CHAR(-.5,4.30,2HP=,2,0.,.1,.1)
      CALL CHAR(-.5,4.60,LPRES,4,0.,.1,.1)
      CALL CHAR(-.5,5.20,2HMM,2,0.,.1,.1)
      CALL CHAR(-.5,5.70,4HOPL=,4,0.,.1,.1)
      ENCODE(4,2503,LOPL) OPL
2503  FORMAT(F4.0)
      CALL CHAR(-.5,6.15,LOPL,4,0.,.1,.1)
      CALL CHAR(-.5,6.75,2HCM,2,0.,.1,.1)
      CALL CHAR(-.5,7.35,6HPOL.=,6,0.,.1,.1)
      ENCODE(5,2504,LPOL) POLANGLE
2504  FORMAT(F5.1)
      CALL CHAR(-.5,7.95,LPOL,5,0.,.1,.1)
      CALL CHAR(-.5,8.65,3HDEG,3,0.,.1,.1)
      CALL PLOT (0.,5.,2)
      CALL PLOT (0.,0.,0)
      CALL PLOT (0.,0.,2,100.,SX)
2600 CONTINUE
      DO 3000 LL=1,IFREQ

```



```

      L=IFREQ+1-LL
      X=XNU(L)
      IF(IOP(15)) GO TO 3001
      Y1=0.1
      CALL PLOT(0.,X,2)
      IF(A(L).LT.0.0) Y1=-0.1
      GO TO 3200
3001  CALL PLOT(0.,X,2,SY,SX)
      Y1=A(L)
3200  CONTINUE
      CALL PLOT(Y1,X,1)
3000  CALL PLOT(0.,X,1)
      CALL PLOT(0.,X,2,SY,SX)
      GO TO NG0
      150  IF(KALL) CALL LINESHAP
           DO 9 K=1,IFREQ
           CALL ARSC0(K)
           9  CONTINUE
           IJ=-XMAX+SX
           IT=-IJ
CALCULATES SLIT FUNCTION
      IF(IOP(1)) CALL SLITFUNC
CALCULATES ROTATION ANGLE/UNIT PATH LENGTH
      IF(IOP(2)) CALL REFRACT
CALCULATES INDIVIDUAL TRANSMISSIONS, PLOTS C.D. PATTERN
      IF(IOP(3)) CALL TRANS
CALCULATES AND/OR PLOTS UNINTEGRATED FARADAY ROTATION
      IF(IOP(4)) 6999,7020
6999  IF(IOP(11)) GO TO 7000
      IF(IOP(4).NE.2) GO TO 7000
      IF(NUMM) 7010,7000
7010  ASSIGN 7000 TO NG0
      CALL PLOT(0.,0.,2,SY,SX)
      CALL PLOT(0.,-5.,2,100.,100.)
      CALL PLOT(0.,0.,0)
      GO TO 9000
7000  CALL FARROT
7020  CONTINUE
C  PLOTS INDIVIDUAL TRANSMISSION CURVES
      IF(IOP(5)) 30,9300
      30  IF(IOP(11)) GO TO 7100
      IF(NUMM) 7110,7100
7110  ASSIGN 7100 TO NG0
      CALL PLOT(0.,0.,2,SY,SX)
      CALL PLOT(0.,-5.,2,100.,100.)
      CALL PLOT(0.,0.,0)
      GO TO 9000
7100  CONTINUE
      X=IJ/SX
      NUMM=1
      CALL PLOT(1.,X,2,SY,SX)
      DO 31 L=IJ,IT
      X=X+(1./SX)
      YT=TRANSM(L)**2

```




```

31 CALL PLOT(YT,X,1,SY,SX)
   X=IJ/SX
   CALL PLOT(1.,X,2,SY,SX)
   DO 32 L=IJ,IT
   X=X+(1./SX)
   YT=TRANSP(L)**2
32 CALL PLOT(YT,X,1,SY,SX)
9300 CONTINUE
CALCULATES AND/OR PLOTS INTEGRATED C.D. PATTERN
   IF(IOP(6)) 9400,9500
9400 CONTINUE
   IF(IOP(11)) GO TO 500
   IF(IOP(6).NE.2) GO TO 500
   IF(NUMM) 7200,500
7200 ASSIGN 500 TO NGO
   CALL PLOT(0.,0.,2,SY,SX)
   CALL PLOT(0.,-5.,2,100.,100.)
   CALL PLOT(0.,0.,0)
   GO TO 9000
500 CONTINUE
   NB=IJ-IMIN
   NT=-NB $ X=NB/SX
   IF(IOP(6).EQ.2) NUMM=1
   CALL PLOT(0.,X,2,SY,SX)
   DO 510 N=NB,NT
   X=X+(1./SX)
   YS=0.
   DO 505 M=IMIN,IMAX
   NM=N+M
505 YS=YS+SHAPE(M)*CD(NM)
   YT=YS/SLITNOHM
   CDINT(N)=YT
   IF(IOP(6).EQ.2) CALL PLOT(YT,X,1,SY,SX)
510 CONTINUE
9500 CONTINUE
CALCULATES AND/OR PLOTS INTEGRATED FARADAY ROTATION
   IF(IOP(7)) 9600,9700
9600 CONTINUE
   IF(IOP(11)) GO TO 7300
   IF(IOP(7).NE.2) GO TO 7300
   IF(NUMM) 7310,7300
7310 ASSIGN 7300 TO NGO
   CALL PLOT(0.,0.,2,SY,SX)
   CALL PLOT(0.,-5.,2,100.,100.)
   CALL PLOT(0.,0.,0)
   GO TO 9000
7300 CONTINUE
   NB=-599-IMIN
   NT=-NB
   X=NB/SX
   IF(IOP(7).EQ.2) NUMM=1
   CALL PLOT(0.,X,2,SY,SX)
   DO 610 N=NB,NT
   X=X+(1./SX)

```



```

      YS=0.
      DO 605 M=IMIN,IMAX
      NM=N+M
605  YS=YS+SHAPE(M)*FARADAY(NM)
      YT=YS/SLITNORM
      FARINT(N)=YT
      IF(IOP(7).EQ.2) CALL PLOT(YT,X,1,SY,SX)
610  CONTINUE
9700 CONTINUE
C   PLOTS INTEGRATED M.R. SIGNAL
      IF(IOP(8)) 9800,9900
9800 CONTINUE
      IF(IOP(11)) GO TO 9802
      IF(NUMM) 9801,9802
9801 ASSIGN 9802 TO NGO
      CALL PLOT(0.,0.,2,SY,SX)
      CALL PLOT(0.,-5.,2,100.,100.)
      CALL PLOT(0.,0.,0)
      GO TO 9000
9802 NUMM=1
      NB=-599-IMIN & NT=-NR & X=NB/SX
      CALL PLOT(0.,X,2,SY,SX)
      DO 710 N=NR,NT
      X=X+(1./SX)
      Y=CDINT(N)+FARINT(N)
710  CALL PLOT(Y,X,1,SY,SX)
9900 CONTINUE
C   PLOTS UNINTEGRATED M.R. SIGNAL
      IF(IOP(9)) 9910,9920
9910 CONTINUE
      IF(IOP(11)) GO TO 9915
      IF(NUMM) 9911,9915
9911 ASSIGN 9915 TO NGO
      CALL PLOT(0.,0.,2,SY,SX)
      CALL PLOT(0.,-5.,2,100.,100.)
      CALL PLOT(0.,0.,0)
      GO TO 9000
9915 NUMM=1
      L=-500
      X=L/SX
      CALL PLOT(0.,X,2,SY,SX)
      DO 810 I=L,500
      X=X+(1./SX)
      Y=CD(I)+FARADAY(I)
810  CALL PLOT(Y,X,1,SY,SX)
9920 CONTINUE
C   PLOTS ABSORPTION
      IF(IOP(12)) 9930,9940
9930 CONTINUE
      IF(IOP(11)) GO TO 7400
      IF(NUMM) 7410,7400
7410 ASSIGN 7400 TO NGO
      CALL PLOT(0.,0.,2,SY,SX)
      CALL PLOT(0.,-5.,2,100.,100.)

```



```

CALL PLOT(0.,0.,0)
GO TO 9000
7400 CONTINUE
NB=-599-IMIN $ NT=-NB $ X=NB/SX
NUMM=1
CALL PLOT(0.,X,2,SY,SX)
DO 9931 J=NB,NT
X=X+(1./SX)
YS=0.
DO 9932 K=IMIN,IMAX
JK=J+K
TM=TRANSM(JK)*TRANSM(JK)
TP=TRANSP(JK)*TRANSP(JK)
9932 YS=YS+SHAPE(K)*(2.-TM-TP)
YT=YS/SLITNORM
9931 CALL PLOT(YT,X,1,SY,SX)
9940 CONTINUE
C PRINTS VALUES OF ALL QUANTITIES
IF(IOP(13)) 9950,9960
9950 CONTINUE
PRINT 9952
9952 FORMAT(*1 X*7X*ABSORPTION* 8X*TRANS.*10X*CD*9X*ROT. ANGLE*10X
1*FR*12X*MR*9X*INT. MR*10X*SF*/)
N=0 $ X=0.
INDEX=5
IF(IOP(13).EQ.2) INDEX=1
IF(IOP(13).EQ.3) INDEX=2
IF(IOP(13).EQ.4) INDEX=10
DO 9951 I=N,600,INDEX
AB=ABSCOFM(I)+ABSCOFF(I)
TR=TRANSM(I)*TRANSP(I)
XMR=CD(I)+FARADAY(I)
XMRI=CDINT(I)+FARINT(I)
PRINT 9955,X,AB,TR,CD(I),PHI(I),FARADAY(I),XMR,XMRI,SHAPE(I)
9955 FORMAT(F10.4,4X,E10.3,4X,2(F10.4,4X),E13.3,4X,4(F10.4,4X))
9951 X=X+(INDEX/SX)
9960 CONTINUE
20 CALL PLOT(0.,0.,2,SY,SX)
CALL PLOT(0.,-5.,2,100.,100.)
CALL PLOT(0.,0.,0)
Y=0.
X=0.
IF(P(NN)) GO TO 1
GO TO 99
80 CALL PLOT (JUB,0.,-1)
100 FORMAT(2F20.2)
102 FORMAT(3A8)
200 FORMAT(*1*,2R1,X,12,*/2 N*12*0*6X,F10.1* GAUSS*)
201 FORMAT(* *4X,F10.4,2X,F10.4)
202 FORMAT(*0*10X,12HVALUES INPUT// *5X,9HFREQUENCY,4X,9HINTENSITY/)
203 FORMAT(*0DOPPLER HALFWIDTH *F10.4* CM-1*)
1203 FORMAT(X*LORENTZ HALFWIDTH *F10.4* CM-1/ATM,*)
204 FORMAT(X*SPECT. HALFWIDTH *F10.4* CM-1*)
205 FORMAT(X*INT. ABSORP. COEF. *F10.5* CM-2/ATM,*)

```



```

206 FORMAT(X*OPTICAL PATHLENGTH *F10.1* CM*)
207 FORMAT(X*PRESSURE*11X,F10.2* TORR*)
208 FORMAT(X*POLARIZER ANGLE*4X,F10.2* DEGREES*)
END

```

SUBROUTINE LINESHAP

```

COMMON/1/ XNU(300),A(300)
COMMON/2/ DABSCOFM(601),ABSCOFM(600),DABSCOFP(601),ABSCOFP(600)
COMMON/3/ SY,SX,MAXPOS,GAML,GAMD, IOP(20),NUMBER,XMAX,NUMM
COMMON/4/ DSHAPE(601),SHAPE(600),IMAX,IMIN,SLITWDTH,POL,SLITTRAP
COMMON/5/ I LABEL(4),FIELD
COMMON/6/ RANGE,HEIGHT,SO,P(8),PRES,OPL,XNUZERO,SLITNORM,TOL
COMMON/7/ DTRMSM(601),TRMSM(600),DTRANSP(601),TRANSP(600),
1DCD(601),CD(600)
COMMON/8/ DPHI(601),PHI(600)
COMMON/9/ DFARADAY(601),FARADAY(600)
COMMON/10/ DCDINT(601),CDINT(600),DFARINT(601),FARINT(600)
COMMON/11/ DLNSHP(601),XLNSHP(600)
IF(.NOT.GAML) GO TO 5000
JMAX=700
DEL=1./SX
TLINE=TOL
NN=1
IF(DEL.GT.TLINE) 500,600
500 TLINE=2.*TLINE
NN=2*NN
IF(DEL.GT.TLINE) 500,510
510 DEL=DEL/NN
JMAX=600*NN+100
600 DDEL=DEL*DEL
GL=GAML*PRES/760. F CON=0.1491*GL*DEL/GAMD $ GGL=GL*GL
SIG=(.694/(GAMD**2))*DDEL
N=0
DO 10 I=N,600
II=I*NN
XL=0.
DO 20 J=N,JMAX
DENOM=GGL+J*J*DDEL
XNUM=EXP(-SIG*((J+II)**2))
X=XNUM/DENOM
XL=XL+X
IF(X.LT.1.E-6) GO TO 21
20 CONTINUE
PRINT 100
21 DO 30 K=1,JMAX
J=K
DENOM=GGL+J*J*DDEL
XNUM=EXP(-SIG*((J+II)**2))
X=XNUM/DENOM
XL=XL+X
IF(II-K) 29,30,30
29 IF(X.LT.1.E-6) GO TO 31
30 CONTINUE
PRINT 100

```




```

31 XLNSHP(I)=XL*CON
   IF(XLNSHP(I).LT.1.E-6) GO TO 40
10  CONTINUE
   PRINT 200
40  IIMAX=I
   DO 50 L=1,IIMAX
     I=L
50  XLNSHP(I)=XLNSHP(L)
     KALL=0
     PRINT 1000,(XLNSHP(I),I=N,500,10)
1000 FORMAT(F20.10)
     RETURN
5000 SIG=.694/((GAMD**2)*SX)
     CON=.47/GAMD
     N=0
     DO 110 I=N,500
       X=EXP(-SIG*(I**2))
       XLNSHP(I)=Y*CON
       IF(XLNSHP(I).LT.1.E-8) GO TO 111
110  CONTINUE
     PRINT 100
111  IIMAX=I
     DO 150 L=1,IIMAX
       I=L
150  XLNSHP(I)=YLNSHP(L)
     KALL=0
     RETURN
100  FORMAT(*HAVE EXCEEDED NO LOOP*)
200  FORMAT(*HAVE EXCEEDED MAIN LOOP*)
END

```

```

SUBROUTINE ARSCO(K)
COMMON/1/ XNU(300),A(300)
COMMON/2/ DABSCOFM(601),ABSCOFM(600),DABSCOFF(601),ABSCOFF(600)
COMMON/3/ SY,SX,MAXPOS,GAML,GAMD, IOP(20),NUMBER,XMAX,NUMM
COMMON/4/ DSHAPE(601),SHAPE(600),IMAX,IMIN,SLITWIDTH,POL,SLITTRAP
COMMON/5/ I LABEL(4),FIELD
COMMON/6/ RANGE,HEIGHT,S0,P(8),PRES,OPL,XNUZERO,SLITNORM,TOL
COMMON/7/ DTRASM(601),TRASM(600),DTRANSP(601),TRANSP(600),
1 DCD(601),CD(600)
COMMON/8/ DPHI(601),PHI(600)
COMMON/9/ DFARADAY(601),FARADAY(600)
COMMON/10/ DCDINT(601),CDINT(600),DFARINT(601),FARINT(600)
COMMON/11/ DLNSHP(601),XLNSHP(600)
AT=A(K)*S0*PRES/760.
ATXL=ABSF(AT*OPL)
X=XNU(K)
TEST=1./SY
DO 10 J=1,599,5
  ABCO=ATXL*XLNSHP(J)
  TEMP=1.-EXP(-ARCO)
  IF(TEMP.LT.TEST) GO TO 12
10  CONTINUE
12  XW=X-J/SX

```



```

      IF (ABSF(XW).GT.XMAX) XMAX=ABSF(XW)
      IN=X+SY
      IW=XW+SX
      MAX=IW+XABSF(2*(IN-IW))
      IT=XABSF(IN)+XABSF(J)
      IF (IT.GT.600 ) 1100,1200
1100 XMAX=600./SX
      IF (IN) 1000,1000,3000
1000 IW=-600
      MAX=600+2*IN
      GO TO 1200
3000 MAX=600
      IW=-600+2*IN
1200 CONTINUE
      DO 20 J=IW,MAX
      IL=J-IN
      Y=AT*XLNSHP(IL)
      IF (Y) 100,20,300
100 ABSCOFM(J)=ABSCOFM(J)+ABSF(Y)
      GO TO 20
300 ABSCOFP(J)=ABSCOFP(J)+Y
20 CONTINUE
      RETURN
      END

```

```

SUBROUTINE SLITFUNC
COMMON/1/ XND(300),A(300)
COMMON/2/ DABSCOFM(601),ABSCOFM(600),DABSCOFP(601),ABSCOFP(600)
COMMON/3/ SY,SX,MAXPOS,GAML,GAMD, IOP(20),NUMBER,XMAX,NUMM
COMMON/4/ DSHAPE(601),SHAPE(600),IMAX,IMIN,SLITWIDTH,POL,SLITIRAP
COMMON/5/ LABEL(4),FIELD
COMMON/6/ RANGE,HEIGHT,S0,P(8),PRES,OPL,XNUZERO,SLITNORM,TOL
COMMON/7/ DTRMSM(601),TRMSM(600),DTRANSP(601),TRANSP(600),
1 DCD(601),CD(600)
COMMON/8/ DPHI(601),PHI(600)
COMMON/9/ DFARADAY(601),FARADAY(600)
COMMON/10/ DCDINT(601),CDINT(600),DFARINT(601),FARINT(600)
COMMON/11/ DLNSHP(601),XLNSHP(600)
TEST=1./SY
IF (IOP(1).EQ.2) GO TO 500
IF (IOP(1).EQ.3) GO TO 700
SLITNORM=SX*SLITWIDTH*2.13
SIG=.694/(SLITWIDTH*2)
N=0
SHAPE(N)=1.0
X=0.
DO 10 I=1,600
X=X+(1./SX)
SHAPE(I)=EXP(-SIG*(X**2))
IF (SHAPE(I).LT.TEST) 20,10
10 CONTINUE
PRINT 100
100 FORMAT(*1A RANGE TOO SMALL FOR THE SLITWIDTH HAS BEEN USED*)
20 IMAX=I $ IMIN=-IMAX

```



```

      PRINT 200, X
200  FORMAT (X*THE HALF-EXTENT OF SLIT FUNCTION IS*F8.4* CM-1*)
      DO 30 J=1,IMAX
      L=J
      SHAPE(L)=SHAPE(J)
30  CONTINUE
      GO TO 1000
500  SLITNORM=SX*SLITWIDTH*2.
      N=0 & SHAPE(N)=1.0
      X=0.
      DO 510 I=1,600
      X=X+(1./SX)
      SHAPE(I)=1.-(.5*X/SLITWIDTH)
      IF(SHAPE(I).LT.TEST) 520,510
510  CONTINUE
      PRINT 100
520  IMAX=I & IMIN=-IMAX
      PRINT 200,X
      DO 530 J=1,IMAX
      L=J
      SHAPE(L)=SHAPE(J)
530  CONTINUE
      GO TO 1000
700  SLITNORM=SX*SLITWIDTH*2.0
      N=0 & X=0. & ITMAX=SLITTRAP*SX
      DO 710 I=N,ITMAX
      X=X+(1./SX)
      SHAPE(I)=1.0
710  CONTINUE
      IT=ITMAX+1
      SLP=SLITWIDTH-SLITTRAP
      DO 720 I=IT,600
      X=X+(1./SX)
      SHAPE(I)=1.-(.5*X/SLP)
      IF(SHAPE(I).LT.TEST) 730,720
720  CONTINUE
      PRINT 100
730  IMAX=I & IMIN=-IMAX
      PRINT 200,X
      DO 740 J=1,IMAX
      L=J
      SHAPE(L)=SHAPE(J)
740  CONTINUE
1000 CONTINUE
      IOP(1)=0
      RETURN
      END

```

SUBROUTINE REFRACT

```

COMMON/1/ XNU(300),A(300)
COMMON/2/ DABSCOFM(601),ABSCOFM(600),DABSCOFF(601),ABSCOFF(600)
COMMON/3/ SY,SX,MAXPOS,GAML,GAMD, IOP(20),NUMBER,XMAX,NUMM
COMMON/4/ DSHAPE(601),SHAPE(600),IMAX,IMIN,SLITWIDTH,POL,SLITTRAP
COMMON/5/ ILABEL(4),FIELD

```



```

COMMON/6/ RANGE,HEIGHT,SQ,P(8),PRES,OPL,XNUZERO,SLITNORM,TOL
COMMON/7/ DTRASM(601),TRANSM(600),DTRANSP(601),TRANSP(600),
1DCD(601),CD(600)
COMMON/8/ DPHI(601),PHI(600)
COMMON/9/ DFARADAY(601),FARADAY(600)
COMMON/10/ DCDINT(601),CDINT(600),DFARINT(601),FARINT(600)
COMMON/11/ DLNSHP(601),XLNSHP(600)
DIMENSION DDIF(600),DIF(600)
IJ=-XMAX*SY
IT=-IJ
N=0
DO 10 L=IJ,IT
10 DIF(L)=ABSCOFM(L)-ABSCOF( L)
CON=1./(4.+3.14159)
DO 20 J=N,599
PT0=.5*(DIF(J+1)-DIF(J-1))
PT=0.
DO 25 I=IJ,IT
IF(I.EQ.J) GO TO 25
PT=PT+DIF(I)/(I-J)
25 CONTINUE
20 PHI(J)=CON*(PT+PT0)
DO 30 J=1,599
K=*J
30 PHI(K)=PHI(J)
RETURN
END

SUBROUTINE TRANS
COMMON/1/ XNU(300),A(300)
COMMON/2/ DABSCOFM(601),ABSCOFM(600),DABSCOF(601),ABSCOF(600)
COMMON/3/ SY,SX,MAXPOS,GAM1,GAM0, IOP(20),NUMBER,XMAX,NUMM
COMMON/4/ DSHAPE(601),SHAPE(600),IMAX,IMIN,SLITWIDTH,POL,SLITRAP
COMMON/5/ LABEL(4),FIELD
COMMON/6/ RANGE,HEIGHT,SQ,P(8),PRES,OPL,XNUZERO,SLITNORM,TOL
COMMON/7/ DTRASM(601),TRANSM(600),DTRANSP(601),TRANSP(600),
1DCD(601),CD(600)
COMMON/8/ DPHI(601),PHI(600)
COMMON/9/ DFARADAY(601),FARADAY(600)
COMMON/10/ DCDINT(601),CDINT(600),DFARINT(601),FARINT(600)
COMMON/11/ DLNSHP(601),XLNSHP(600)
IJ=-XMAX*SY
IT=-IJ
X=IJ/SX
ASSIGN 10 TO NG0
IF(IOP(3).EQ.2) 500,600
500 CALL PLOT(0.,X,2,SY,SX)
NUMM=1
ASSIGN 110 TO NG0
600 DO 10 L=IJ,IT
X=X+(1./SX)
TM=(ABSCOFM(L)*OPL)/2.
TP=(ABSCOF( L)*OPL)/2.
TRANSM(L)=EXP(-TM)

```




```

TRANSP(L)=EXP(-TP)
IF(TRANSM(L).LT.1.E-100) TRANSM(L)=0.
IF(TRANSP(L).LT.1.E-100) TRANSP(L)=0.
CD(L)=(TRANSM(L)-TRANSP(L))*2/4.
GO TO NGO
110 CALL PLOT(CD(L),X,1)
10 CONTINUE
RETURN
END

SUBROUTINE FARROT
COMMON/1/ XNU(300),A(300)
COMMON/2/ DABSCOFM(601),ABSCOFM(600),DABSCOFF(601),ABSCOFF(600)
COMMON/3/ SY,SX,MAXPOS,GAML,GAMD, IOP(20),NUMBER,XMAX,NUMM
COMMON/4/ DSHAPE(601),SHAPE(600),IMAX,IMIN,SLITWIDTH,POL,SLITTRAP
COMMON/5/ ILABEL(4),FIELD
COMMON/6/ RANGE,HEIGHT,S0,P(8),PRES,OPL,XNUZERO,SLITNORM,TOL
COMMON/7/ DTRANSM(601),TRANSM(600),DTRANSP(601),TRANSP(600),
1 DCD(601),CD(600)
COMMON/8/ DPHI(601),PHI(600)
COMMON/9/ DFARADAY(601),FARADAY(600)
COMMON/10/ DCDINT(601),CDINT(600),DFARINT(601),FARINT(600)
COMMON/11/ DLNSHP(601),XLNSHP(600)
N=0
DO 10 J=N,599
X=OPL*PHI(J)+POL
SN=(SINF(X))*2
XX=TRANSM(J)+TRANSP(J)
10 FARADAY(J)=SN*XX
DO 20 K=1,599
J=-K
20 FARADAY(J)=FARADAY(K)
IF(IOP(4).NE.2) RETURN
NUMM=1
L=-500
X=L/SX
CALL PLOT(FARADAY(L),X,2,SY,SX)
DO 30 K=L,500
CALL PLOT(FARADAY(K),X,1,SY,SX)
30 X=X+1./SX
RETURN
END

```

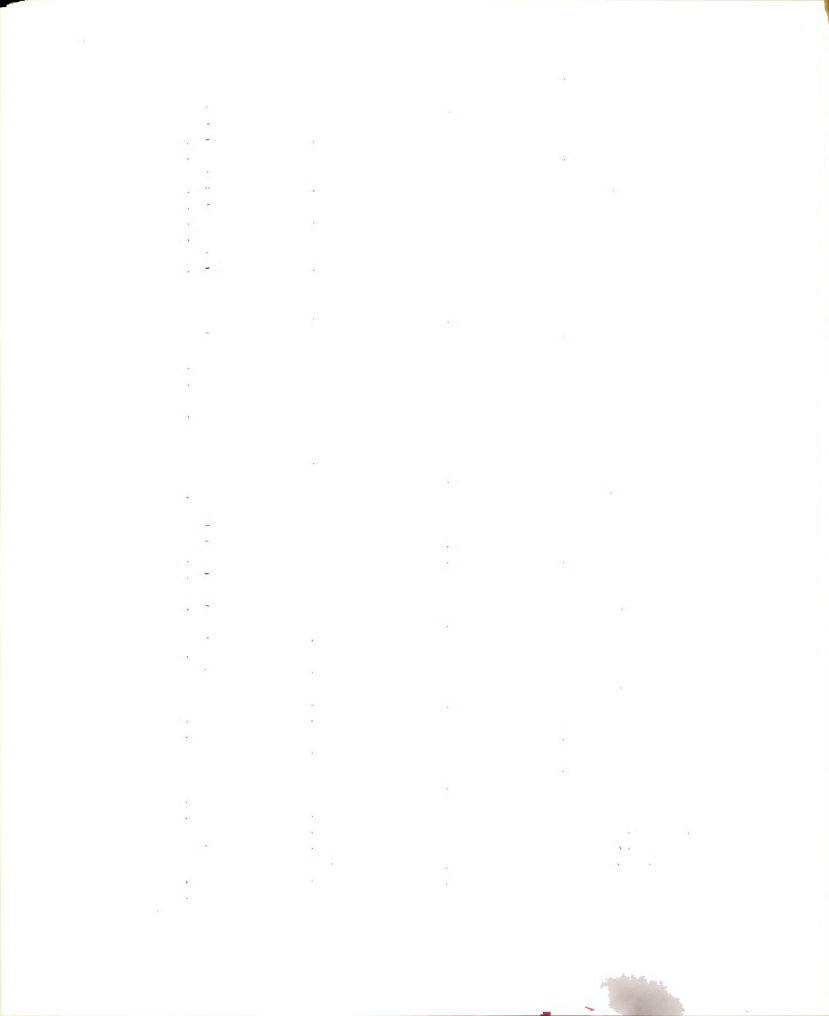


APPENDIX VIII-A

GROUND STATE COMBINATION DIFFERENCE FIT FOR $^{14}\text{N}^{16}\text{O}$

DEL					WGT.	OBS.	PRED.	(O-P)
N	S	V	J	J				
1	2	0	1	7/2	0.00	15,5088	15,4766	0,0322
2	2	0	1	9/2	0.00	18,8957	18,9137	-0,0180
3	2	0	1	13/2	0.45	25,7884	25,7838	0,0046
4	2	0	1	15/2	0.00	29,2080	29,2164	-0,0084
5	2	0	1	17/2	0.00	32,6486	32,6471	0,0015
6	2	0	1	21/2	0.00	39,5050	39,5018	0,0032
7	2	0	1	23/2	0.00	42,9153	42,9253	-0,0100
8	2	0	2	5/2	0.80	27,5128	27,5150	-0,0022
9	2	0	2	7/2	2.00	34,3930	34,3903	0,0027
10	2	0	2	9/2	2.00	41,2639	41,2632	0,0007
11	2	0	2	11/2	2.00	48,1382	48,1334	0,0048
12	2	0	2	13/2	2.00	55,0015	55,0003	0,0012
13	2	0	2	15/2	2.00	61,8636	61,8635	0,0001
14	2	0	2	17/2	3.91	68,7263	68,7227	0,0036
15	2	0	2	19/2	2.40	75,5783	75,5774	0,0009
16	2	0	2	21/2	2.65	82,4288	82,4271	0,0017
17	2	0	2	23/2	2.00	89,2735	89,2715	0,0020
18	2	0	2	25/2	2.00	96,1112	96,1102	0,0010
19	2	0	2	27/2	2.05	102,9425	102,9428	-0,0003
20	2	0	2	29/2	2.07	109,7659	109,7689	-0,0030
21	2	0	2	31/2	0.00	116,5903	116,5883	0,0020
22	2	0	2	33/2	2.00	123,3991	123,4005	-0,0014
23	2	0	2	35/2	2.67	130,2025	130,2054	-0,0029
24	2	0	2	37/2	2.00	137,0010	137,0025	-0,0015
25	2	0	2	39/2	2.00	143,7910	143,7916	-0,0006
26	2	0	2	41/2	1.54	150,5671	150,5725	-0,0054
27	2	0	2	43/2	2.00	157,3424	157,3449	-0,0025
28	2	0	2	45/2	0.80	164,1065	164,1086	-0,0021
29	2	0	2	47/2	1.11	170,8638	170,8635	0,0003
30	2	0	2	49/2	1.03	177,6128	177,6094	0,0034
31	2	0	2	51/2	1.33	184,3452	184,3462	-0,0010
32	2	0	2	53/2	1.33	191,0731	191,0737	-0,0006
33	2	0	2	55/2	1.33	197,7962	197,7919	0,0043
34	2	0	2	59/2	0.00	211,1806	211,2003	-0,0197
35	2	0	2	61/2	0.44	217,8931	217,8905	0,0026

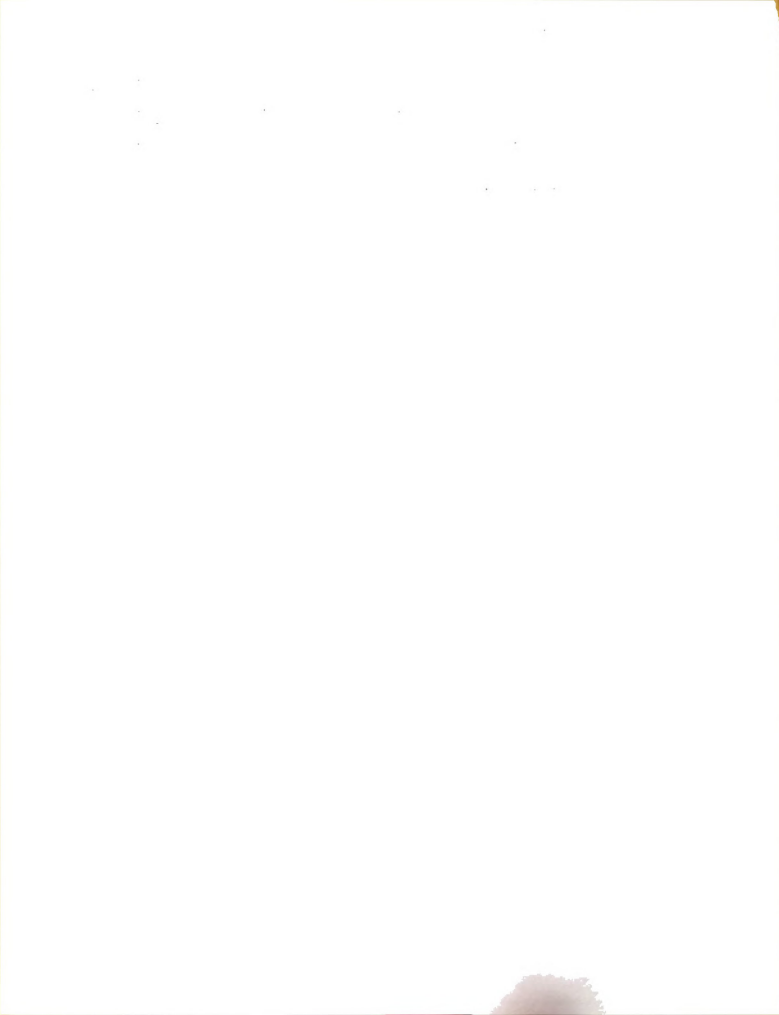
36	2	0	2	63/2	0.46	224,5773	224,5713	0,0060
37	2	0	2	65/2	0.00	231,2435	231,2430	0,0005
38	2	0	2	67/2	0.00	237,8608	237,9055	=0,0447
39	2	0	2	69/2	1.44	244,5585	244,5591	=0,0006
40	1	0	1	1/2	4.44	5,0109	5,0165	=0,0056
41	1	0	1	3/2	7.19	8,3645	8,3608	0,0037
42	1	0	1	5/2	9.29	11,7037	11,7050	=0,0013
43	1	0	1	7/2	5.99	15,0449	15,0491	=0,0042
44	1	0	1	9/2	4.33	18,3922	18,3931	=0,0009
45	1	0	1	11/2	4.38	21,7368	21,7369	=0,0001
46	1	0	1	13/2	4.53	25,0740	25,0805	=0,0065
47	1	0	1	15/2	3.43	28,4238	28,4239	=0,0001
48	1	0	1	17/2	4.53	31,7664	31,7669	=0,0005
49	1	0	1	19/2	3.15	35,1067	35,1097	=0,0030
50	1	0	1	21/2	4.86	38,4527	38,4520	0,0007
51	1	0	1	23/2	3.37	41,7943	41,7939	0,0004
52	1	0	1	25/2	2.48	45,1351	45,1352	=0,0001
53	1	0	1	27/2	4.02	48,4791	48,4760	0,0031
54	1	0	1	29/2	3.43	51,8164	51,8161	0,0003
55	1	0	1	31/2	3.08	55,1594	55,1555	0,0039
56	1	0	1	33/2	0.11	58,5008	58,4940	0,0068
57	1	0	1	35/2	0.59	61,8383	61,8315	0,0068
58	1	0	1	37/2	0.23	65,1691	65,1680	0,0011
59	1	0	1	39/2	0.21	68,5089	68,5033	0,0056
60	1	0	1	41/2	0.00	71,8436	71,8372	0,0064
61	1	0	2	1/2	6.49	13,3770	13,3773	=0,0003
62	1	0	2	3/2	4.38	20,0689	20,0658	0,0031
63	1	0	2	5/2	2.00	26,7511	26,7541	=0,0030
64	1	0	2	7/2	2.00	33,4398	33,4422	=0,0024
65	1	0	2	9/2	3.30	40,1269	40,1300	=0,0031
66	1	0	2	11/2	2.00	46,8150	46,8174	=0,0024
67	1	0	2	13/2	2.00	53,5011	53,5044	=0,0033
68	1	0	2	15/2	2.94	60,1896	60,1908	=0,0012
69	1	0	2	17/2	2.67	66,8753	66,8766	=0,0013
70	1	0	2	19/2	3.61	73,5613	73,5617	=0,0004
71	1	0	2	21/2	2.40	80,2440	80,2459	=0,0019
72	1	0	2	23/2	2.80	86,9284	86,9291	=0,0007
73	1	0	2	25/2	2.71	93,6102	93,6113	=0,0011
74	1	0	2	27/2	2.35	100,2959	100,2921	0,0038
75	1	0	2	29/2	2.00	106,9757	106,9716	0,0041
76	1	0	2	31/2	2.00	113,6508	113,6494	0,0014
77	1	0	2	33/2	2.00	120,3317	120,3255	0,0062
78	1	0	2	35/2	2.40	127,0052	126,9995	0,0057
79	1	0	2	37/2	2.00	133,6732	133,6712	0,0020
80	1	0	2	39/2	0.00	140,3340	140,3405	=0,0065
81	1	0	2	41/2	0.00	147,0000	147,0069	=0,0069
82	1	0	2	43/2	1.33	153,6709	153,6703	0,0006
83	1	0	2	45/2	1.54	160,3331	160,3303	0,0028
84	1	0	2	47/2	1.54	166,9848	166,9865	=0,0017
85	1	0	2	49/2	1.11	173,6407	173,6386	0,0021
86	1	0	2	51/2	1.39	180,2830	180,2862	=0,0032
87	1	0	2	53/2	1.33	186,9201	186,9288	=0,0087
88	1	0	2	55/2	1.33	193,5584	193,5660	=0,0076
89	1	0	2	57/2	1.33	200,1914	200,1974	=0,0060



222

90	1	0	2	59/2	0.54	206,8169	206,8224	-0,0055
91	1	0	2	63/2	0.00	220,0403	220,0511	-0,0108
92	1	0	2	65/2	0.46	226,6589	226,6535	0,0054
93	1	0	2	67/2	0.54	233,2465	233,2472	-0,0007
94	1	0	2	69/2	0.00	239,8322	239,8315	0,0007
95	1	0	2	71/2	0.89	246,4155	246,4057	0,0098

S.D. = 0,0032



FREQUENCY FIT FOR 14N160 INPUTING GSCD CONSTANTS

N	V	LINE	WGT.	OBSERVED	PREDICTED	(O-P)
1	1	P1 3/2	2.00	1871.0621	1871.0644	-0.0023
2	1	P1 5/2	2.00	1867.6678	1867.6686	-0.0008
3	1	P1 7/2	2.00	1864.2372	1864.2387	-0.0015
4	1	P1 9/2	2.00	1860.7738	1860.7745	-0.0007
5	1	P1 11/2	2.00	1857.2751	1857.2761	-0.0010
6	1	P1 13/2	2.00	1853.7426	1853.7436	-0.0010
7	1	P1 15/2	2.00	1850.1777	1850.1769	0.0008
8	1	P1 17/2	2.00	1846.5784	1846.5761	0.0023
9	1	P1 19/2	2.00	1842.9420	1842.9412	0.0008
10	1	P1 21/2	2.00	1839.2729	1839.2722	0.0007
11	1	P1 23/2	2.00	1835.5705	1835.5692	0.0013
12	1	P1 25/2	2.00	1831.8345	1831.8322	0.0023
13	1	P1 27/2	2.00	1828.0622	1828.0612	0.0010
14	1	P1 29/2	2.00	1824.2581	1824.2563	0.0018
15	1	P1 31/2	2.00	1820.4175	1820.4175	-0.0000
16	1	P1 33/2	2.00	1816.5447	1816.5449	-0.0002
17	1	P1 35/2	2.00	1812.6403	1812.6386	0.0017
18	1	P1 37/2	2.00	1808.6959	1808.6985	-0.0026
19	1	P1 39/2	3.00	1804.7237	1804.7249	-0.0012
20	1	P1 41/2	2.00	1800.7203	1800.7177	0.0026
21	1	P1 43/2	0.00	1796.6884	1796.6771	0.0113
22	1	P1 45/2	0.00	1792.6158	1792.6031	0.0127
23	1	P1 47/2	1.00	1788.4977	1788.4960	0.0017
24	1	P1 49/2	1.25	1784.3583	1784.3558	0.0025
25	1	P1 51/2	1.25	1780.1857	1780.1826	0.0031
26	1	P1 53/2	1.25	1775.9811	1775.9767	0.0044
27	1	P1 55/2	1.06	1771.7412	1771.7382	0.0030
28	1	P1 57/2	1.00	1767.4719	1767.4673	0.0046
29	1	P1 59/2	1.00	1763.1680	1763.1641	0.0039
30	1	P1 61/2	1.00	1758.8344	1758.8290	0.0054
31	1	P1 63/2	0.31	1754.4648	1754.4621	0.0027
32	1	P1 67/2	0.00	1745.6376	1745.6343	0.0033
33	1	P1 69/2	0.25	1741.1611	1741.1738	-0.0127
34	1	P1 71/2	0.31	1736.6771	1736.6828	-0.0057
35	1	P1 73/2	0.80	1732.1552	1732.1615	-0.0063
36	1	P1 75/2	0.50	1727.5964	1727.6104	-0.0140
37	1	P2 5/2	1.25	1867.2154	1867.2050	0.0104
38	1	P2 7/2	2.00	1863.6850	1863.6762	0.0088
39	1	P2 9/2	2.00	1860.1206	1860.1123	0.0083
40	1	P2 11/2	2.00	1856.5204	1856.5135	0.0069
41	1	P2 13/2	2.00	1852.8884	1852.8801	0.0083
42	1	P2 15/2	2.00	1849.2157	1849.2122	0.0035
43	1	P2 17/2	2.00	1845.5164	1845.5102	0.0062
44	1	P2 19/2	2.00	1841.7786	1841.7743	0.0043
45	1	P2 21/2	2.00	1838.0078	1838.0046	0.0032
46	1	P2 23/2	2.00	1834.2044	1834.2014	0.0030
47	1	P2 25/2	2.00	1830.3675	1830.3650	0.0025
48	1	P2 27/2	2.00	1826.4956	1826.4954	0.0002
49	1	P2 29/2	2.00	1822.5922	1822.5930	-0.0008

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272	273	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370	371	372	373	374	375	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442	443	444	445	446	447	448	449	450	451	452	453	454	455	456	457	458	459	460	461	462	463	464	465	466	467	468	469	470	471	472	473	474	475	476	477	478	479	480	481	482	483	484	485	486	487	488	489	490	491	492	493	494	495	496	497	498	499	500	501	502	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521	522	523	524	525	526	527	528	529	530	531	532	533	534	535	536	537	538	539	540	541	542	543	544	545	546	547	548	549	550	551	552	553	554	555	556	557	558	559	560	561	562	563	564	565	566	567	568	569	570	571	572	573	574	575	576	577	578	579	580	581	582	583	584	585	586	587	588	589	590	591	592	593	594	595	596	597	598	599	600	601	602	603	604	605	606	607	608	609	610	611	612	613	614	615	616	617	618	619	620	621	622	623	624	625	626	627	628	629	630	631	632	633	634	635	636	637	638	639	640	641	642	643	644	645	646	647	648	649	650	651	652	653	654	655	656	657	658	659	660	661	662	663	664	665	666	667	668	669	670	671	672	673	674	675	676	677	678	679	680	681	682	683	684	685	686	687	688	689	690	691	692	693	694	695	696	697	698	699	700	701	702	703	704	705	706	707	708	709	710	711	712	713	714	715	716	717	718	719	720	721	722	723	724	725	726	727	728	729	730	731	732	733	734	735	736	737	738	739	740	741	742	743	744	745	746	747	748	749	750	751	752	753	754	755	756	757	758	759	760	761	762	763	764	765	766	767	768	769	770	771	772	773	774	775	776	777	778	779	780	781	782	783	784	785	786	787	788	789	790	791	792	793	794	795	796	797	798	799	800	801	802	803	804	805	806	807	808	809	810	811	812	813	814	815	816	817	818	819	820	821	822	823	824	825	826	827	828	829	830	831	832	833	834	835	836	837	838	839	840	841	842	843	844	845	846	847	848	849	850	851	852	853	854	855	856	857	858	859	860	861	862	863	864	865	866	867	868	869	870	871	872	873	874	875	876	877	878	879	880	881	882	883	884	885	886	887	888	889	890	891	892	893	894	895	896	897	898	899	900	901	902	903	904	905	906	907	908	909	910	911	912	913	914	915	916	917	918	919	920	921	922	923	924	925	926	927	928	929	930	931	932	933	934	935	936	937	938	939	940	941	942	943	944	945	946	947	948	949	950	951	952	953	954	955	956	957	958	959	960	961	962	963	964	965	966	967	968	969	970	971	972	973	974	975	976	977	978	979	980	981	982	983	984	985	986	987	988	989	990	991	992	993	994	995	996	997	998	999	1000	1001	1002	1003	1004	1005	1006	1007	1008	1009	1010	1011	1012	1013	1014	1015	1016	1017	1018	1019	1020	1021	1022	1023	1024	1025	1026	1027	1028	1029	1030	1031	1032	1033	1034	1035	1036	1037	1038	1039	1040	1041	1042	1043	1044	1045	1046	1047	1048	1049	1050	1051	1052	1053	1054	1055	1056	1057	1058	1059	1060	1061	1062	1063	1064	1065	1066	1067	1068	1069	1070	1071	1072	1073	1074	1075	1076	1077	1078	1079	1080	1081	1082	1083	1084	1085	1086	1087	1088	1089	1090	1091	1092	1093	1094	1095	1096	1097	1098	1099	1100	1101	1102	1103	1104	1105	1106	1107	1108	1109	1110	1111	1112	1113	1114	1115	1116	1117	1118	1119	1120	1121	1122	1123	1124	1125	1126	1127	1128	1129	1130	1131	1132	1133	1134	1135	1136	1137	1138	1139	1140	1141	1142	1143	1144	1145	1146	1147	1148	1149	1150	1151	1152	1153	1154	1155	1156	1157	1158	1159	1160	1161	1162	1163	1164	1165	1166	1167	1168	1169	1170	1171	1172	1173	1174	1175	1176	1177	1178	1179	1180	1181	1182	1183	1184	1185	1186	1187	1188	1189	1190	1191	1192	1193	1194	1195	1196	1197	1198	1199	1200	1201	1202	1203	1204	1205	1206	1207	1208	1209	1210	1211	1212	1213	1214	1215	1216	1217	1218	1219	1220	1221	1222	1223	1224	1225	1226	1227	1228	1229	1230	1231	1232	1233	1234	1235	1236	1237	1238	1239	1240	1241	1242	1243	1244	1245	1246	1247	1248	1249	1250	1251	1252	1253	1254	1255	1256	1257	1258	1259	1260	1261	1262	1263	1264	1265	1266	1267	1268	1269	1270	1271	1272	1273	1274	1275	1276	1277	1278	1279	1280	1281	1282	1283	1284	1285	1286	1287	1288	1289	1290	1291	1292	1293	1294	1295	1296	1297	1298	1299	1300	1301	1302	1303	1304	1305	1306	1307	1308	1309	1310	1311	1312	1313	1314	1315	1316	1317	1318	1319	1320	1321	1322	1323	1324	1325	1326	1327	1328	1329	1330	1331	1332	1333	1334	1335	1336	1337	1338	1339	1340	1341	1342	1343	1344	1345	1346	1347	1348	1349	1350	1351	1352	1353	1354	1355	1356	1357	1358	1359	1360	1361	1362	1363	1364	1365	1366	1367	1368	1369	1370	1371	1372	1373	1374	1375	1376	1377	1378	1379	1380	1381	1382	1383	1384	1385	1386	1387	1388	1389	1390	1391	1392	1393	1394	1395	1396	1397	1398	1399	1400	1401	1402	1403	1404	1405	1406	1407	1408	1409	1410	1411	1412	1413	1414	1415	1416	1417	1418	1419	1420	1421	1422	1423	1424	1425	1426	1427	1428	1429	1430	1431	1432	1433	1434	1435	1436	1437	1438	1439	1440	1441	1442	1443	1444	1445	1446	1447	1448	1449	1450	1451	1452	1453	1454	1455	1456	1457	1458	1459	1460	1461	1462	1463	1464	1465	1466	1467	1468	1469	1470	1471	1472	1473	1474	1475	1476	1477	1478	1479	1480	1481	1482	1483	1484	1485	1486	1487	1488	1489	1490	1491	1492	1493	1494	1495	14
---	---	---	---	---	---	---	---	---	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	----

50	1	P2	31/2	2.00	1818,6562	1818,6580	=0,0018
51	1	P2	33/2	2.00	1814,6895	1814,6904	=0,0009
52	1	P2	35/2	0.00	1810,6848	1810,6906	=0,0058
53	1	P2	37/2	2.00	1806,6560	1806,6586	=0,0026
54	1	P2	39/2	4.00	1802,5904	1802,5947	=0,0043
55	1	P2	41/2	2.00	1798,4906	1798,4990	=0,0084
56	1	P2	43/2	2.00	1794,3653	1794,3716	=0,0063
57	1	P2	45/2	1.25	1790,2101	1790,2127	=0,0026
58	1	P2	47/2	2.00	1786,0183	1786,0224	=0,0041
59	1	P2	49/2	0.50	1781,7936	1781,8008	=0,0072
60	1	P2	51/2	1.25	1777,5433	1777,5480	=0,0047
61	1	P2	53/2	1.06	1773,2571	1773,2641	=0,0070
62	1	P2	55/2	1.00	1768,9423	1768,9491	=0,0068
63	1	P2	57/2	1.00	1764,5973	1764,6031	=0,0058
64	1	P2	59/2	1.00	1760,2179	1760,2260	=0,0081
65	1	P2	63/2	0.00	1751,3985	1751,3790	0,0195
66	1	P2	65/2	0.25	1746,9073	1746,9089	=0,0016
67	1	P2	67/2	0.25	1742,4046	1742,4077	=0,0031
68	1	P2	69/2	0.25	1737,8741	1737,8754	=0,0013
69	1	P2	71/2	0.00	1733,3576	1733,3118	0,0458
70	1	P2	73/2	0.87	1728,7216	1728,7168	0,0048
71	1	R1	1/2	2.00	1881,0430	1881,0459	=0,0029
72	1	R1	3/2	0.12	1884,3080	1884,3044	0,0036
73	1	R1	5/2	2.00	1887,5249	1887,5286	=0,0037
74	1	R1	7/2	2.00	1890,7149	1890,7183	=0,0034
75	1	R1	9/2	2.00	1893,8708	1893,8735	=0,0027
76	1	R1	11/2	2.00	1896,9927	1896,9943	=0,0016
77	1	R1	13/2	2.00	1900,0795	1900,0804	=0,0009
78	1	R1	15/2	2.00	1903,1310	1903,1320	=0,0010
79	1	R1	17/2	4.00	1906,1482	1906,1488	=0,0006
80	1	R1	19/2	3.00	1909,1314	1909,1308	0,0006
81	1	R1	21/2	3.00	1912,0785	1912,0781	0,0004
82	1	R1	23/2	3.00	1914,9911	1914,9903	0,0008
83	1	R1	25/2	2.00	1917,8670	1917,8676	=0,0006
84	1	R1	27/2	2.00	1920,7128	1920,7097	0,0031
85	1	R1	29/2	2.00	1923,5204	1923,5165	0,0039
86	1	R1	31/2	2.00	1926,2911	1926,2880	0,0031
87	1	R1	33/2	2.00	1929,0276	1929,0240	0,0036
88	1	R1	35/2	2.00	1931,7289	1931,7244	0,0045
89	1	R1	37/2	2.00	1934,3935	1934,3889	0,0046
90	1	R1	39/2	2.00	1937,0224	1937,0176	0,0048
91	1	R1	41/2	2.00	1939,6158	1939,6101	0,0057
92	1	R1	43/2	2.00	1942,1686	1942,1663	0,0023
93	1	R1	45/2	2.00	1944,6914	1944,6861	0,0053
94	1	R1	47/2	2.00	1947,1705	1947,1691	0,0014
95	1	R1	49/2	1.00	1949,6218	1949,6153	0,0065
96	1	R1	51/2	2.00	1952,0242	1952,0244	=0,0002
97	1	R1	53/2	2.00	1954,3920	1954,3961	=0,0041
98	1	R1	55/2	2.00	1956,7264	1956,7302	=0,0038
99	1	R1	57/2	2.00	1959,0258	1959,0265	=0,0007
100	1	R1	59/2	2.00	1961,2817	1961,2846	=0,0029
101	1	R1	63/2	2.00	1965,6779	1965,6854	=0,0075
102	1	R1	65/2	3.00	1967,8200	1967,8274	=0,0074
103	1	R1	67/2	2.00	1969,9236	1969,9301	=0,0065

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

100

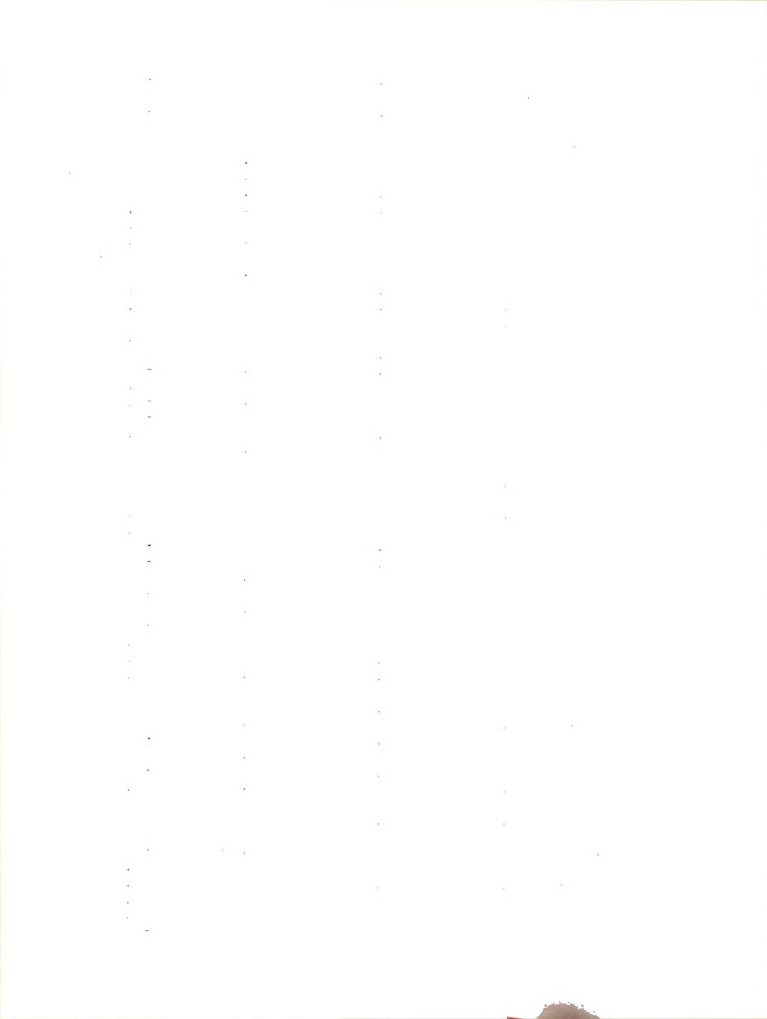
100

100

100

100

104	1	R1	69/2	0.00	1971,9874	1971,9931	=0,0057
105	1	R1	71/2	4.25	1974,0119	1974,0162	=0,0043
106	1	R1	73/2	4.06	1975,9970	1975,9989	=0,0019
107	1	R1	77/2	3.27	1979,8486	1979,8417	0,0069
108	1	R1	79/2	1.02	1981,7183	1981,7011	0,0172
109	1	R1	81/2	0.25	1983,5390	1983,5185	0,0205
110	1	R1	83/2	0.03	1985,3251	1985,2936	0,0315
111	1	R2	5/2	0.50	1887,6334	1887,6273	0,0061
112	1	R2	7/2	2.00	1890,9134	1890,9038	0,0096
113	1	R2	9/2	2.00	1894,1523	1894,1433	0,0090
114	1	R2	11/2	2.00	1897,3539	1897,3456	0,0083
115	1	R2	13/2	2.00	1900,5179	1900,5105	0,0074
116	1	R2	15/2	2.00	1903,6422	1903,6378	0,0044
117	1	R2	17/2	4.00	1906,7335	1906,7273	0,0062
118	1	R2	19/2	3.00	1909,7827	1909,7788	0,0039
119	1	R2	21/2	3.00	1912,7972	1912,7921	0,0051
120	1	R2	23/2	2.00	1915,7691	1915,7669	0,0022
121	1	R2	25/2	2.00	1918,7034	1918,7032	0,0002
122	1	R2	27/2	2.00	1921,5985	1921,6007	=0,0022
123	1	R2	29/2	2.00	1924,4551	1924,4593	=0,0042
124	1	R2	31/2	2.00	1927,2751	1927,2789	=0,0038
125	1	R2	33/2	2.00	1930,0551	1930,0591	=0,0040
126	1	R2	35/2	2.00	1932,7929	1932,8000	=0,0071
127	1	R2	37/2	2.00	1935,4916	1935,5014	=0,0098
128	1	R2	39/2	2.00	1938,1563	1938,1632	=0,0069
129	1	R2	41/2	2.00	1940,7772	1940,7852	=0,0080
130	1	R2	43/2	2.00	1943,3607	1943,3673	=0,0066
131	1	R2	45/2	2.00	1945,9001	1945,9094	=0,0093
132	1	R2	47/2	1.00	1948,4071	1948,4115	=0,0044
133	1	R2	49/2	1.00	1950,8699	1950,8735	=0,0036
134	1	R2	51/2	2.00	1953,2875	1953,2952	=0,0077
135	1	R2	53/2	2.00	1955,6704	1955,6767	=0,0063
136	1	R2	55/2	2.00	1958,0141	1958,0179	=0,0038
137	1	R2	57/2	2.00	1960,3188	1960,3188	0,0000
138	1	R2	59/2	2.00	1962,5791	1962,5792	=0,0001
139	1	R2	61/2	2.00	1964,8004	1964,7993	0,0011
140	1	R2	63/2	3.00	1966,9819	1966,9790	0,0029
141	1	R2	67/2	5.00	1971,2184	1971,2173	0,0011
142	1	R2	69/2	4.25	1973,2801	1973,2758	0,0043
143	1	R2	71/2	4.06	1975,2977	1975,2941	0,0036
144	1	R2	73/2	4.06	1977,2728	1977,2722	0,0006
145	1	R2	75/2	2.52	1979,2082	1979,2101	=0,0019
146	1	R2	79/2	0.25	1982,9551	1982,9656	=0,0105
147	1	R2	81/2	0.03	1984,7701	1984,7834	=0,0133
148	1	PH	5/2	3.50	1987,3424	1987,3585	=0,0161
149	1	PH	7/2	4.25	1984,1496	1984,1631	=0,0135
150	1	PH	13/2	0.81	1974,9266	1974,9277	=0,0011
151	1	PH	19/2	0.59	1966,2034	1966,1980	0,0054
152	1	PH	21/2	0.00	1963,3488	1963,3943	=0,0455
153	1	PH	23/2	0.83	1960,6465	1960,6409	0,0056
154	1	PH	27/2	0.22	1955,2907	1955,2772	0,0135
155	1	PH	29/2	0.50	1952,6705	1952,6629	0,0076
156	1	PH	31/2	0.19	1950,0931	1950,0904	0,0027
157	1	QH	3/2	3.44	1995,7093	1995,7192	=0,0099



158	1	QH	5/2	3.44	1995,8561	1995,8681	=0,0120
159	1	QH	7/2	5.75	1996,0692	1996,0758	=0,0066
160	1	QH	9/2	5.75	1996,3367	1996,3416	=0,0049
161	1	QH	11/2	6.50	1996,6594	1996,6646	=0,0052
162	1	QH	13/2	4.25	1997,0403	1997,0437	=0,0034
163	1	QH	15/2	6.25	1997,4819	1997,4776	0,0043
164	1	QH	17/2	7.25	1997,9706	1997,9649	0,0057
165	1	QH	19/2	7.25	1998,5101	1998,5039	0,0062
166	1	QH	21/2	5.25	1999,1019	1999,0928	0,0091
167	1	QH	23/2	7.25	1999,7395	1999,7297	0,0098
168	1	QH	25/2	6.71	2000,4216	2000,4125	0,0091
169	1	QH	27/2	5.71	2001,1481	2001,1389	0,0092
170	1	QH	29/2	6.25	2001,9131	2001,9065	0,0066
171	1	QH	31/2	6.25	2002,7202	2002,7131	0,0071
172	1	QH	33/2	6.52	2003,5586	2003,5559	0,0027
173	1	QH	35/2	0.06	2004,4293	2004,4324	=0,0031
174	1	QH	37/2	5.47	2005,3351	2005,3399	=0,0048
175	1	QH	39/2	2.02	2006,2678	2006,2757	=0,0079
176	1	QH	41/2	0.75	2007,2268	2007,2372	=0,0104
177	1	QH	43/2	0.37	2008,2061	2008,2214	=0,0153
178	1	QH	45/2	0.12	2009,2108	2009,2259	=0,0151
179	1	QH	47/2	0.02	2010,2235	2010,2478	=0,0243
180	1	RH	1/2	6.25	2000,7202	2000,7357	=0,0155
181	1	RH	3/2	4.06	2004,2184	2004,2289	=0,0105
182	1	RH	5/2	5.25	2007,7710	2007,7808	=0,0098
183	1	RH	7/2	6.25	2011,3816	2011,3907	=0,0091
184	1	RH	9/2	3.25	2015,0516	2015,0577	=0,0061
185	1	RH	11/2	2.25	2018,7790	2018,7806	=0,0016
186	1	RH	13/2	2.25	2022,5563	2022,5581	=0,0018
187	1	RH	15/2	2.25	2026,3944	2026,3888	0,0056
188	1	RH	17/2	2.25	2030,2763	2030,2709	0,0054
189	1	RH	19/2	2.25	2034,2086	2034,2025	0,0061
190	1	RH	21/2	2.25	2038,1911	2038,1817	0,0094
191	1	RH	23/2	2.25	2042,2159	2042,2064	0,0095
192	1	RH	25/2	1.25	2046,2841	2046,2741	0,0100
193	1	RH	27/2	2.06	2050,3927	2050,3826	0,0101
194	1	RH	29/2	2.02	2054,5361	2054,5292	0,0069
195	1	RH	31/2	2.02	2058,7180	2058,7113	0,0067
196	1	RH	33/2	0.50	2062,9301	2062,9263	0,0038
197	1	RH	35/2	0.31	2067,1735	2067,1714	0,0021
198	1	RH	37/2	0.12	2071,4369	2071,4437	=0,0068
199	1	RH	39/2	0.12	2075,7358	2075,7404	=0,0046
200	1	RH	41/2	0.00	2080,0497	2080,0587	=0,0090
201	1	PL	7/2	0.02	1743,7736	1743,7518	0,0218
202	1	PL	9/2	0.00	1739,8602	1739,8601	0,0001
203	1	PL	11/2	0.33	1735,8506	1735,8411	0,0095
204	1	PL	13/2	0.14	1731,7099	1731,6960	0,0139
205	1	PL	15/2	0.45	1727,4296	1727,4259	0,0037
206	1	PL	17/2	0.00	1723,0406	1723,0325	0,0081
207	1	PL	19/2	0.00	1718,5314	1718,5175	0,0139
208	1	PL	21/2	0.89	1713,8731	1713,8825	=0,0094
209	1	PL	23/2	2.35	1709,1216	1709,1298	=0,0082
210	1	PL	25/2	0.41	1704,2579	1704,2613	=0,0034
211	1	PL	29/2	0.31	1694,1797	1694,1865	=0,0068

212	1	PL	31/2	0.06	1688.9736	1688.9851	-0.0115
213	1	PL	33/2	0.31	1683.6705	1683.6777	-0.0072
214	1	PL	35/2	0.06	1678.2606	1678.2672	-0.0066
215	1	QL	3/2	0.00	1756.1344	1756.1146	0.0198
216	1	QL	7/2	0.37	1755.3554	1755.3367	0.0187
217	1	QL	9/2	0.00	1754.7463	1754.7548	-0.0085
218	1	QL	13/2	0.16	1753.2180	1753.2098	0.0082
219	1	QL	15/2	0.00	1752.2486	1752.2490	-0.0004
220	1	QL	17/2	0.00	1751.1800	1751.1646	0.0154
221	1	QL	21/2	0.00	1748.6199	1748.6315	-0.0116
222	1	QL	23/2	0.00	1747.1732	1747.1866	-0.0134
223	1	RL	7/2	0.00	1770.2551	1770.2314	0.0237
224	1	RL	17/2	2.08	1782.6006	1782.6053	-0.0047
225	1	RL	21/2	0.18	1786.6781	1786.6884	-0.0103
226	1	RL	27/2	0.04	1791.9257	1791.9278	-0.0021
227	1	RL	29/2	0.04	1793.4459	1793.4467	-0.0008

S.D. = 0.0065

APPENDIX VIII-B

GROUND STATE COMBINATION DIFFERENCE FIT FOR 15N16O

DEL					WGT.	OBS.	PRED.	(O-P)
N	S	V	J	J				
1	1	0	1	1/2	1.00	4,8429	4,8418	0,0011
2	1	0	1	3/2	0.68	8,0673	8,0696	-0,0023
3	1	0	1	5/2	2.18	11,2901	11,2973	-0,0072
4	1	0	1	7/2	3.59	14,5262	14,5249	0,0013
5	1	0	1	9/2	2.67	17,7559	17,7523	0,0036
6	1	0	1	11/2	4.94	20,9792	20,9796	-0,0004
7	1	0	1	13/2	2.42	24,2039	24,2066	-0,0027
8	1	0	1	15/2	1.49	27,4327	27,4334	-0,0007
9	1	0	1	17/2	3.00	30,6579	30,6599	-0,0020
10	1	0	1	19/2	2.74	33,8824	33,8859	-0,0035
11	1	0	1	21/2	2.67	37,1118	37,1116	0,0002
12	1	0	1	23/2	1.78	40,3365	40,3368	-0,0003
13	1	0	1	25/2	0.72	43,5676	43,5614	0,0062
14	1	0	1	27/2	2.67	46,7858	46,7855	0,0003
15	1	0	1	29/2	0.89	50,0139	50,0088	0,0051
16	1	0	1	31/2	0.23	53,2276	53,2314	-0,0038
17	1	0	1	35/2	0.04	59,6744	59,6739	0,0005
18	1	0	1	37/2	0.00	62,8878	62,8936	-0,0058
19	1	0	2	1/2	2.68	12,9071	12,9114	-0,0043
20	1	0	2	5/2	0.80	25,8223	25,8222	0,0001
21	1	0	2	7/2	2.00	32,2769	32,2772	-0,0003
22	1	0	2	9/2	1.69	38,7247	38,7320	-0,0073
23	1	0	2	11/2	2.00	45,1835	45,1863	-0,0028
24	1	0	2	13/2	2.00	51,6308	51,6401	-0,0093
25	1	0	2	15/2	2.00	58,0887	58,0933	-0,0046
26	1	0	2	17/2	2.14	64,5441	64,5458	-0,0017
27	1	0	2	19/2	2.00	71,0020	70,9975	0,0045
28	1	0	2	21/2	2.00	77,4426	77,4484	-0,0058
29	1	0	2	23/2	2.00	83,9015	83,8982	0,0033
30	1	0	2	25/2	2.00	90,3481	90,3469	0,0012
31	1	0	2	27/2	2.00	96,7960	96,7943	0,0017
32	1	0	2	29/2	2.40	103,2312	103,2402	-0,0090
33	1	0	2	31/2	1.33	109,6903	109,6845	0,0058
34	1	0	2	33/2	0.80	116,1280	116,1270	0,0010
35	1	0	2	35/2	2.00	122,5677	122,5674	0,0003

36	1	0	2	37/2	1.54	129,0145	129,0057	0,0088
37	1	0	2	39/2	1.39	135,4534	135,4415	0,0119
38	1	0	2	41/2	1.33	141,8769	141,8746	0,0023
39	1	0	2	43/2	0.00	148,3080	148,3048	0,0032
40	1	0	2	45/2	0.80	154,7355	154,7317	0,0038
41	1	0	2	47/2	0.54	161,1580	161,1550	0,0030
42	1	0	2	49/2	1.39	167,5793	167,5745	0,0048
43	1	0	2	51/2	1.03	173,9878	173,9897	0,0019
44	1	0	2	53/2	1.39	180,4014	180,4003	0,0011
45	1	0	2	55/2	0.00	186,7935	186,8059	0,0124
46	1	0	2	57/2	0.00	193,2074	193,2061	0,0013
47	1	0	2	59/2	1.33	199,5898	199,6004	0,0106
48	1	0	2	61/2	0.00	205,9870	205,9884	0,0014
49	1	0	2	63/2	0.00	212,3904	212,3696	0,0208
50	1	0	2	67/2	1.90	225,1080	225,1092	0,0012
51	1	0	2	69/2	0.00	231,5062	231,4666	0,0396
52	1	0	2	71/2	0.19	237,8236	237,8148	0,0088
53	2	0	1	5/2	2.00	11,6097	11,6074	0,0023
54	2	0	1	7/2	0.00	14,9253	14,9225	0,0028
55	2	0	1	13/2	0.00	24,7937	24,8614	0,0677
56	2	0	1	15/2	0.44	28,1714	28,1715	0,0001
57	2	0	1	17/2	0.00	31,4802	31,4799	0,0003
58	2	0	1	19/2	0.38	34,7920	34,7863	0,0057
59	2	0	1	21/2	0.57	38,0861	38,0905	0,0044
60	2	0	1	27/2	0.00	47,9772	47,9886	0,0114
61	2	0	2	5/2	0.00	26,5254	26,5299	0,0045
62	2	0	2	7/2	0.00	33,1269	33,1592	0,0323
63	2	0	2	9/2	2.00	39,7871	39,7864	0,0007
64	2	0	2	11/2	2.00	46,4139	46,4111	0,0028
65	2	0	2	13/2	2.00	53,0349	53,0329	0,0020
66	2	0	2	15/2	2.00	59,6518	59,6514	0,0004
67	2	0	2	17/2	2.00	66,2638	66,2661	0,0023
68	2	0	2	19/2	0.80	72,8835	72,8768	0,0067
69	2	0	2	21/2	2.00	79,4805	79,4830	0,0025
70	2	0	2	23/2	2.00	86,0813	86,0844	0,0031
71	2	0	2	25/2	2.00	92,6750	92,6805	0,0055
72	2	0	2	27/2	2.67	99,2700	99,2712	0,0012
73	2	0	2	29/2	2.40	105,8534	105,8560	0,0026
74	2	0	2	31/2	1.33	112,4393	112,4346	0,0047
75	2	0	2	33/2	2.00	119,0052	119,0067	0,0015
76	2	0	2	35/2	1.54	125,5706	125,5720	0,0014
77	2	0	2	37/2	0.50	132,1308	132,1303	0,0005
78	2	0	2	39/2	0.67	138,6845	138,6813	0,0032
79	2	0	2	41/2	0.44	145,2241	145,2247	0,0006
80	2	0	2	43/2	1.39	151,7599	151,7604	0,0005
81	2	0	2	45/2	0.80	158,2898	158,2881	0,0017
82	2	0	2	47/2	0.54	164,8074	164,8077	0,0003
83	2	0	2	49/2	1.39	171,3214	171,3189	0,0025
84	2	0	2	51/2	0.00	177,8485	177,8217	0,0268
85	2	0	2	53/2	0.54	184,3203	184,3159	0,0044
86	2	0	2	55/2	1.39	190,8109	190,8015	0,0094
87	2	0	2	57/2	0.73	197,2805	197,2783	0,0022
88	2	0	2	59/2	0.32	203,7513	203,7464	0,0049
89	2	0	2	63/2	0.00	216,6528	216,6562	0,0034

230

90	2	0	2	67/2	0.71	229,5218	229,5311	=0,0093
91	2	0	2	71/2	0.12	242,3417	242,3718	=0,0301

S.D. = 0,0044

FREQUENCY FIT FOR 15N160 INPUTING GSCD CONSTANTS

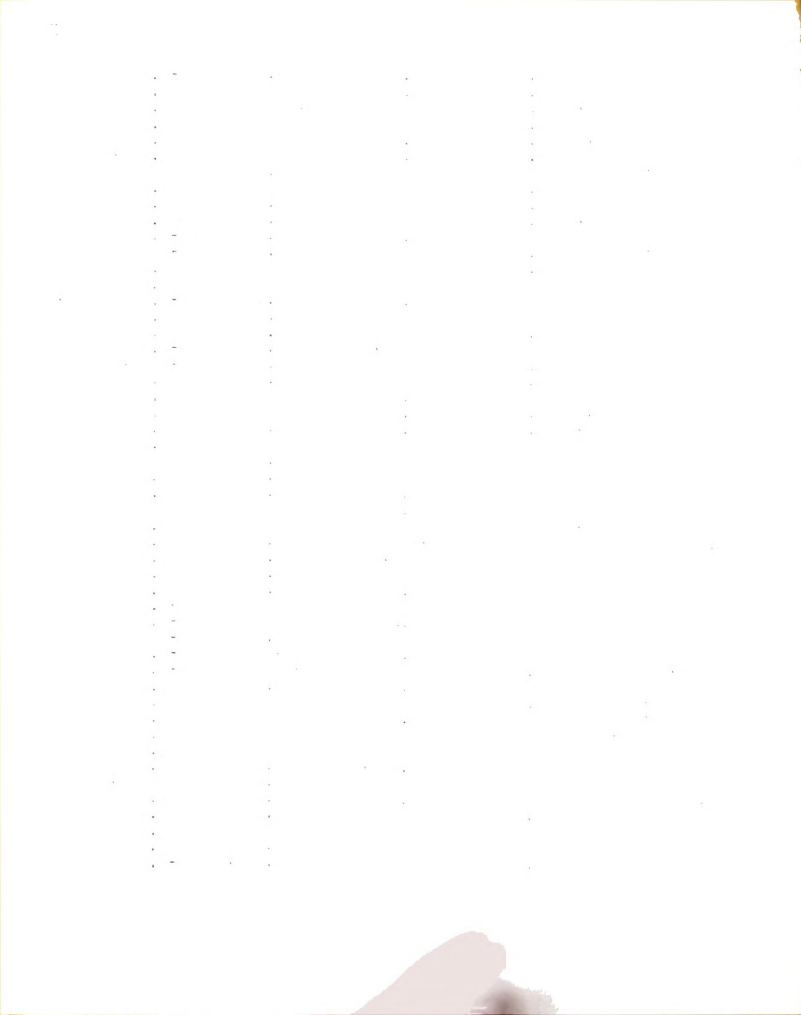
N	V	LINE	WGT,	OBSERVED	PREDICTED	(O-P)
1	1	P1 77/2	0.50	1695.7322	1695.7341	=0.0019
2	1	P1 75/2	0.12	1700.1321	1700.1370	=0.0049
3	1	P1 73/2	0.00	1704.4740	1704.5111	=0.0371
4	1	P1 71/2	4.00	1708.8576	1708.8562	0.0014
5	1	P1 67/2	0.00	1717.4356	1717.4584	=0.0228
6	1	P1 65/2	0.00	1721.7132	1721.7151	=0.0019
7	1	P1 63/2	1.00	1725.9500	1725.9419	0.0081
8	1	P1 61/2	0.00	1730.1360	1730.1385	=0.0025
9	1	P1 59/2	0.00	1734.3142	1734.3048	0.0094
10	1	P1 57/2	1.06	1738.4392	1738.4407	=0.0015
11	1	P1 55/2	1.06	1742.5464	1742.5459	0.0005
12	1	P1 53/2	1.06	1746.6172	1746.6203	=0.0031
13	1	P1 51/2	0.31	1750.6611	1750.6638	=0.0027
14	1	P1 49/2	0.50	1754.6751	1754.6761	=0.0010
15	1	P1 47/2	0.00	1758.6554	1758.6573	=0.0019
16	1	P1 45/2	1.00	1762.6093	1762.6072	0.0021
17	1	P1 43/2	1.06	1766.5163	1766.5256	=0.0093
18	1	P1 41/2	1.25	1770.4089	1770.4125	=0.0036
19	1	P1 39/2	2.00	1774.2697	1774.2678	0.0019
20	1	P1 37/2	2.00	1778.0889	1778.0914	=0.0025
21	1	P1 35/2	2.00	1781.8808	1781.8832	=0.0024
22	1	P1 33/2	2.00	1785.6504	1785.6432	0.0072
23	1	P1 31/2	2.00	1789.3694	1789.3712	=0.0018
24	1	P1 29/2	2.00	1793.0696	1793.0673	0.0023
25	1	P1 27/2	2.00	1796.7309	1796.7313	=0.0004
26	1	P1 25/2	2.00	1800.3657	1800.3633	0.0024
27	1	P1 23/2	2.00	1803.9610	1803.9631	=0.0021
28	1	P1 21/2	2.00	1807.5305	1807.5308	=0.0003
29	1	P1 19/2	2.00	1811.0696	1811.0662	0.0034
30	1	P1 17/2	2.00	1814.5759	1814.5694	0.0065
31	1	P1 15/2	2.00	1818.0386	1818.0404	=0.0018
32	1	P1 13/2	2.00	1821.4766	1821.4790	=0.0024
33	1	P1 11/2	2.00	1824.8814	1824.8853	=0.0039
34	1	P1 9/2	2.00	1828.2559	1828.2592	=0.0033
35	1	P1 7/2	2.00	1831.5973	1831.6007	=0.0034
36	1	P1 5/2	2.00	1834.9074	1834.9097	=0.0023
37	1	P1 3/2	2.00	1838.1834	1838.1863	=0.0029
38	1	R1 1/2	2.00	1847.8135	1847.8211	=0.0076
39	1	R1 5/2	0.50	1854.0782	1854.0813	=0.0031
40	1	R1 7/2	2.00	1857.1583	1857.1625	=0.0042
41	1	R1 9/2	0.50	1860.2025	1860.2109	=0.0084
42	1	R1 11/2	2.00	1863.2221	1863.2266	=0.0045
43	1	R1 13/2	2.00	1866.2067	1866.2095	=0.0028
44	1	R1 15/2	2.00	1869.1583	1869.1595	=0.0012
45	1	R1 17/2	2.00	1872.0747	1872.0766	=0.0019
46	1	R1 19/2	2.00	1874.9630	1874.9606	0.0024
47	1	R1 21/2	2.00	1877.8083	1877.8117	=0.0034
48	1	R1 23/2	2.00	1880.6324	1880.6295	0.0029
49	1	R1 25/2	2.00	1883.4177	1883.4142	0.0035

50	1	R1	27/2	2.00	1886,1654	1886,1655	0,0001
51	1	R1	29/2	3.00	1888,8816	1888,8833	0,0017
52	1	R1	31/2	1.00	1891,5711	1891,5677	0,0034
53	1	R1	33/2	0.50	1894,2169	1894,2183	0,0014
54	1	R1	35/2	2.00	1896,8374	1896,8352	0,0022
55	1	R1	37/2	2.00	1899,4234	1899,4182	0,0052
56	1	R1	39/2	2.00	1901,9697	1901,9671	0,0026
57	1	R1	41/2	2.00	1904,4862	1904,4818	0,0044
58	1	R1	43/2	2.00	1906,9634	1906,9621	0,0013
59	1	R1	45/2	2.00	1909,4106	1909,4078	0,0028
60	1	R1	47/2	2.00	1911,8191	1911,8188	0,0003
61	1	R1	49/2	2.00	1914,1965	1914,1948	0,0017
62	1	R1	51/2	1.00	1916,5342	1916,5356	0,0014
63	1	R1	53/2	2.00	1918,8406	1918,8410	0,0004
64	1	R1	55/2	2.00	1921,1077	1921,1108	0,0031
65	1	R1	57/2	1.00	1923,3434	1923,3446	0,0012
66	1	R1	59/2	2.00	1925,5398	1925,5423	0,0025
67	1	R1	61/2	2.00	1927,7002	1927,7036	0,0034
68	1	R1	63/2	2.00	1929,8260	1929,8280	0,0020
69	1	R1	65/2	2.00	1931,9140	1931,9154	0,0014
70	1	R1	67/2	1.25	1933,9656	1933,9654	0,0002
71	1	R1	69/2	1.25	1935,9802	1935,9776	0,0026
72	1	R1	71/2	0.50	1937,9557	1937,9518	0,0039
73	1	R1	75/2	0.00	1941,8065	1941,7841	0,0224
74	1	P2	75/2	0.12	1696,8332	1696,8139	0,0193
75	1	P2	73/2	0.50	1701,2654	1701,2549	0,0105
76	1	P2	71/2	0.50	1705,6775	1705,6667	0,0108
77	1	P2	67/2	0.00	1714,4074	1714,4026	0,0048
78	1	P2	65/2	0.00	1718,7343	1718,7267	0,0076
79	1	P2	63/2	0.19	1723,0202	1723,0216	0,0014
80	1	P2	61/2	1.37	1727,2815	1727,2873	0,0058
81	1	P2	59/2	1.06	1731,5179	1731,5237	0,0058
82	1	P2	57/2	0.31	1735,7232	1735,7308	0,0076
83	1	P2	55/2	0.00	1739,8789	1739,9086	0,0297
84	1	P2	53/2	1.06	1744,0501	1744,0570	0,0069
85	1	P2	51/2	0.31	1748,1706	1748,1759	0,0053
86	1	P2	49/2	0.50	1752,2571	1752,2652	0,0081
87	1	P2	47/2	1.06	1756,3202	1756,3249	0,0047
88	1	P2	45/2	0.25	1760,3483	1760,3548	0,0065
89	1	P2	43/2	1.00	1764,3489	1764,3548	0,0059
90	1	P2	41/2	1.25	1768,3187	1768,3248	0,0061
91	1	P2	39/2	1.25	1772,2598	1772,2646	0,0048
92	1	P2	37/2	2.00	1776,1782	1776,1742	0,0040
93	1	P2	35/2	2.00	1780,0440	1780,0534	0,0094
94	1	P2	33/2	2.00	1783,8990	1783,9019	0,0029
95	1	P2	31/2	2.00	1787,7169	1787,7197	0,0028
96	1	P2	29/2	2.00	1791,5102	1791,5066	0,0036
97	1	P2	27/2	2.00	1795,2653	1795,2624	0,0029
98	1	P2	25/2	2.00	1798,9888	1798,9869	0,0019
99	1	P2	23/2	0.50	1802,6814	1802,6800	0,0014
100	1	P2	21/2	2.00	1806,3468	1806,3414	0,0054
101	1	P2	19/2	2.00	1809,9735	1809,9710	0,0025
102	1	P2	17/2	2.00	1813,5698	1813,5685	0,0013
103	1	P2	15/2	2.00	1817,1362	1817,1337	0,0025

104	1	P2	13/2	2.00	1820,6702	1820,6666	0,0036
105	1	P2	11/2	0.00	1824,1794	1824,1667	0,0127
106	1	P2	9/2	2.00	1827,6382	1827,6340	0,0042
107	1	P2	7/2	2.00	1831,0739	1831,0683	0,0056
108	1	P2	5/2	2.00	1834,4720	1834,4692	0,0028
109	1	R2	5/2	0.00	1854,1636	1854,1639	=0,0003
110	1	R2	7/2	0.00	1857,3063	1857,3259	=0,0196
111	1	R2	9/2	2.00	1860,4573	1860,4530	0,0043
112	1	R2	11/2	2.00	1863,5501	1863,5449	0,0052
113	1	R2	13/2	2.00	1866,6047	1866,6014	0,0033
114	1	R2	15/2	2.00	1869,6253	1869,6223	0,0030
115	1	R2	17/2	2.00	1872,6106	1872,6075	0,0031
116	1	R2	19/2	2.00	1875,5649	1875,5568	0,0081
117	1	R2	21/2	2.00	1878,4693	1878,4699	=0,0006
118	1	R2	23/2	2.00	1881,3466	1881,3468	=0,0002
119	1	R2	25/2	2.00	1884,1852	1884,1872	=0,0020
120	1	R2	27/2	4.00	1886,9869	1886,9909	=0,0040
121	1	R2	29/2	3.00	1889,7524	1889,7579	=0,0055
122	1	R2	31/2	1.00	1892,4833	1892,4879	=0,0046
123	1	R2	33/2	2.00	1895,1834	1895,1809	0,0025
124	1	R2	35/2	2.00	1897,8304	1897,8367	=0,0063
125	1	R2	37/2	0.31	1900,4495	1900,4551	=0,0056
126	1	R2	39/2	0.50	1903,0334	1903,0361	=0,0027
127	1	R2	41/2	2.00	1905,5724	1905,5795	=0,0071
128	1	R2	43/2	2.00	1908,0801	1908,0853	=0,0052
129	1	R2	45/2	2.00	1910,5469	1910,5533	=0,0064
130	1	R2	47/2	2.00	1912,9780	1912,9835	=0,0055
131	1	R2	49/2	2.00	1915,3715	1915,3759	=0,0044
132	1	R2	51/2	2.00	1917,7274	1917,7303	=0,0029
133	1	R2	53/2	2.00	1920,0435	1920,0467	=0,0032
134	1	R2	55/2	2.00	1922,3288	1922,3252	0,0036
135	1	R2	57/2	0.50	1924,5620	1924,5656	=0,0036
136	1	R2	59/2	1.00	1926,7715	1926,7680	0,0035
137	1	R2	63/2	2.00	1931,0602	1931,0588	0,0014
138	1	R2	65/2	1.25	1933,1533	1933,1472	0,0061
139	1	R2	67/2	1.25	1935,1993	1935,1978	0,0015
140	1	R2	71/2	0.12	1939,1749	1939,1856	=0,0107
141	1	PL	29/2	0.06	1663,5706	1663,5802	=0,0096
142	1	PL	25/2	0.25	1673,1964	1673,2099	=0,0135
143	1	PL	23/2	0.33	1677,8582	1677,8654	=0,0072
144	1	PL	21/2	0.31	1682,4009	1682,4120	=0,0111
145	1	PL	19/2	0.50	1686,8447	1686,8477	=0,0030
146	1	PL	17/2	0.25	1691,1701	1691,1710	=0,0009
147	1	PL	15/2	0.00	1695,4485	1695,3800	0,0685
148	1	PL	13/2	0.00	1699,4708	1699,4733	=0,0025
149	1	PL	11/2	2.00	1703,4600	1703,4497	0,0103
150	1	PL	9/2	0.00	1707,3133	1707,3080	0,0053
151	1	PL	7/2	2.00	1711,0583	1711,0471	0,0112
152	1	PL	3/2	0.00	1718,1864	1718,1648	0,0216
153	1	QL	31/2	0.50	1708,0992	1708,1137	=0,0145
154	1	QL	27/2	0.00	1711,5478	1711,5688	=0,0210
155	1	QL	21/2	2.00	1715,9443	1715,9559	=0,0116
156	1	QL	19/2	0.50	1717,1929	1717,1982	=0,0053
157	1	QL	17/2	0.00	1718,3249	1718,3276	=0,0027

158	1	QL	15/2	2.00	1719,3415	1/19,3425	=0,0010
159	1	QL	13/2	2.00	1720,2422	1/20,2414	0,0008
160	1	QL	7/2	2.00	1722,2386	1/22,2305	0,0081
161	1	QL	5/2	2.00	1722,6680	1/22,6545	0,0135
162	1	RL	7/2	0.00	1736,6579	1/36,6089	0,0490
163	1	RL	27/2	0.06	1757,8669	1/57,8816	=0,0147
164	1	PH	21/2	0.04	1931,4675	1/31,4602	0,0073
165	1	PH	19/2	0.00	1934,2000	1/34,1894	0,0106
166	1	PH	15/2	0.00	1939,8185	1/39,7941	0,0244
167	1	PH	13/2	0.50	1942,6763	1/42,6722	0,0041
168	1	PH	11/2	0.00	1945,5907	1/45,6023	=0,0116
169	1	PH	9/2	0.52	1948,5692	1/48,5852	=0,0160
170	1	PH	7/2	1.50	1951,6154	1/51,6218	=0,0064
171	1	PH	5/2	0.52	1954,7006	1/54,7127	=0,0121
172	1	QH	3/2	1.00	1962,7679	1/62,7822	=0,0143
173	1	QH	5/2	4.00	1962,9055	1/62,9191	=0,0136
174	1	QH	7/2	4.00	1963,0996	1/63,1101	=0,0105
175	1	QH	9/2	4.00	1963,3476	1/63,3546	=0,0070
176	1	QH	11/2	4.00	1963,6441	1/63,6518	=0,0077
177	1	QH	13/2	5.00	1963,9958	1/64,0008	=0,0050
178	1	QH	15/2	3.06	1964,4011	1/64,4004	0,0007
179	1	QH	17/2	1.19	1964,8510	1/64,8493	0,0017
180	1	QH	19/2	3.00	1965,3521	1/65,3461	0,0060
181	1	QH	21/2	4.00	1965,8982	1/65,8893	0,0089
182	1	QH	23/2	4.00	1966,4860	1/66,4771	0,0089
183	1	QH	25/2	1.60	1967,1174	1/67,1077	0,0097
184	1	QH	27/2	0.47	1967,7831	1/67,7791	0,0040
185	1	QH	29/2	4.00	1968,5015	1/68,4893	0,0122
186	1	QH	31/2	4.00	1969,2411	1/69,2362	0,0049
187	1	QH	33/2	2.00	1970,0260	1/70,0174	0,0086
188	1	QH	37/2	0.50	1971,6784	1/71,6737	0,0047
189	1	QH	39/2	0.12	1972,5484	1/72,5441	0,0043
190	1	QH	41/2	0.03	1973,4387	1/73,4394	=0,0007
191	1	RH	1/2	1.00	1967,6108	1/67,6240	=0,0132
192	1	RH	7/2	2.00	1977,8723	1/77,8795	=0,0072
193	1	RH	9/2	2.00	1981,4000	1/81,4042	=0,0042
194	1	RH	11/2	2.00	1984,9774	1/84,9804	=0,0030
195	1	RH	13/2	2.00	1988,6050	1/88,6070	=0,0020
196	1	RH	15/2	2.00	1992,2837	1/92,2827	0,0010
197	1	RH	17/2	2.00	1996,0100	1/96,0060	0,0040
198	1	RH	19/2	2.00	1999,7806	1/99,7753	0,0053
199	1	RH	21/2	2.00	2003,5978	2/03,5887	0,0091
200	1	RH	23/2	2.00	2007,4539	2/07,4445	0,0094
201	1	RH	25/2	1.54	2011,3507	2/11,3406	0,0101
202	1	RH	27/2	2.00	2015,2872	2/15,2748	0,0124
203	1	RH	29/2	0.50	2019,2551	2/19,2450	0,0101
204	1	RH	31/2	0.12	2023,2536	2/23,2487	0,0049
205	1	RH	33/2	0.02	2027,2882	2/27,2838	0,0044
206	1	RH	35/2	0.02	2031,3528	2/31,3476	0,0052
207	1	RH	37/2	0.00	2035,4363	2/35,4377	=0,0014

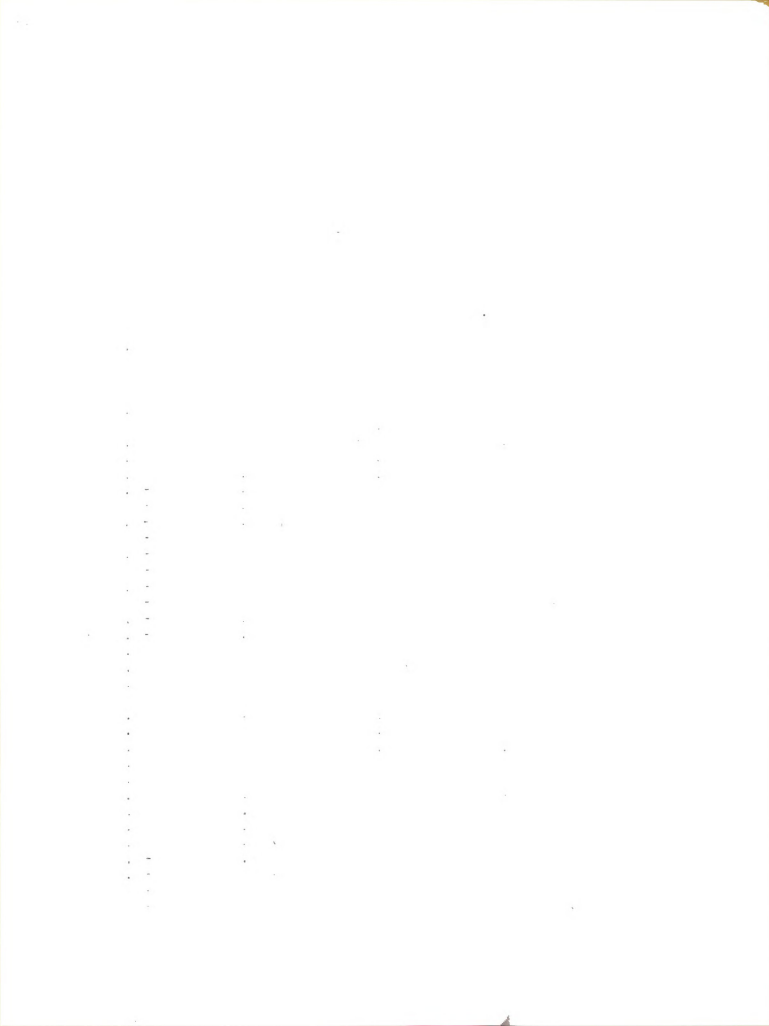
S.D. = 0,0059



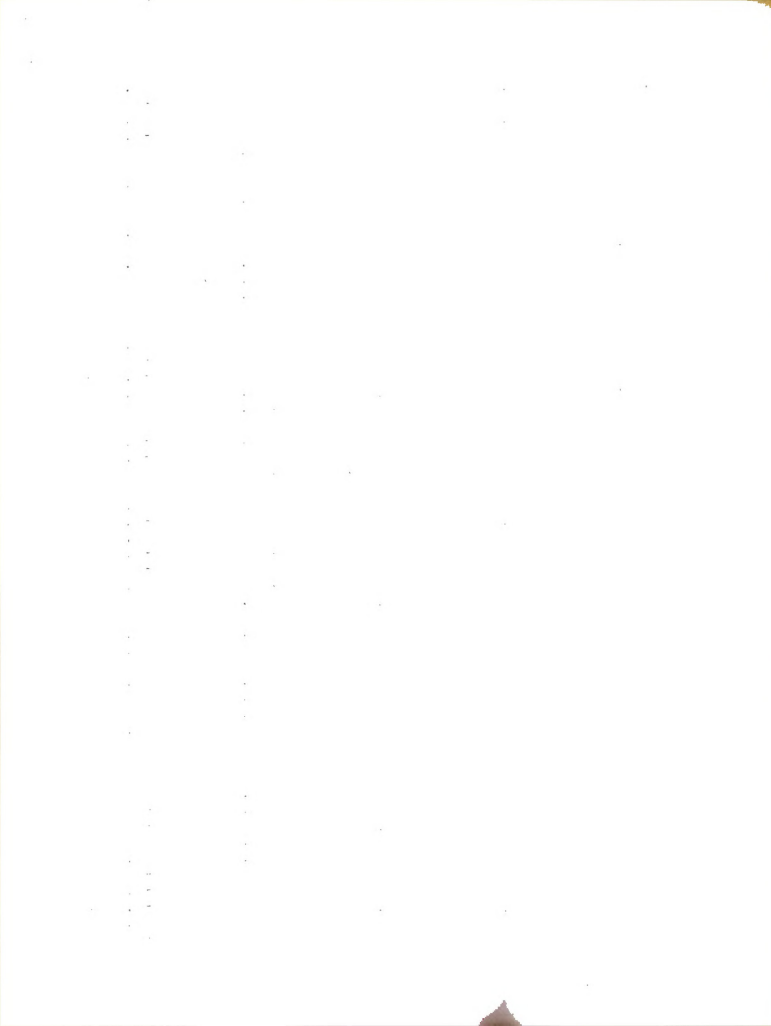
APPENDIX IX-A

FREQUENCY FIT FOR 14N160

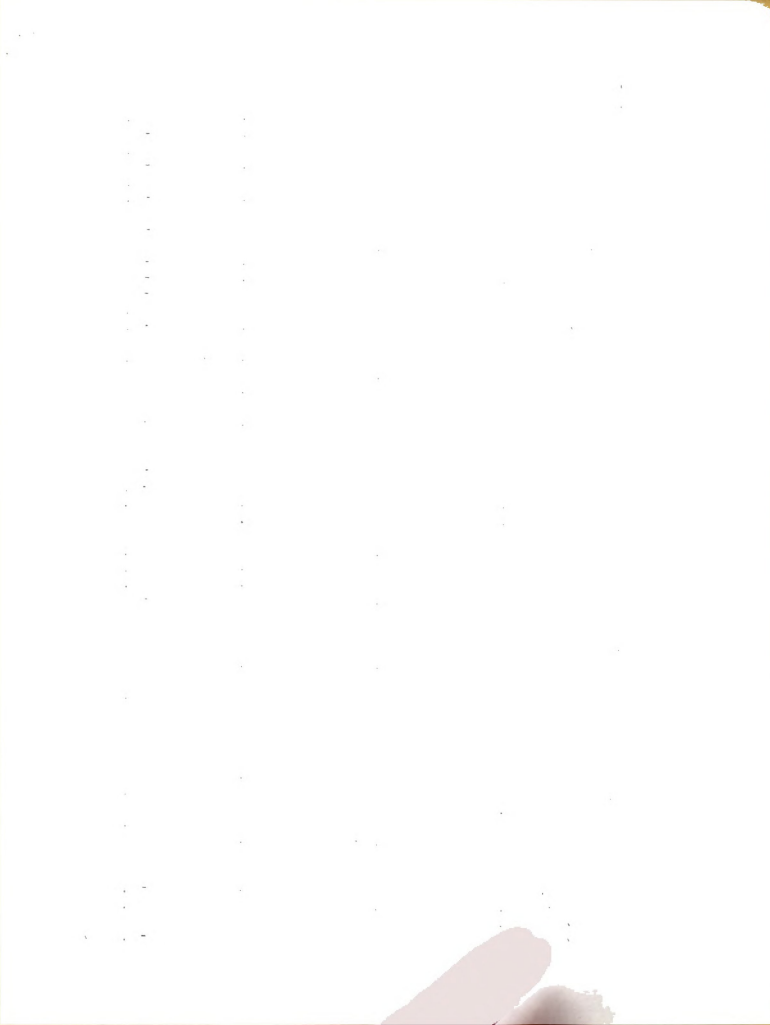
N	V	LINE	WGT,	OBSERVED	PREDICTED	(O-P)
1	1	P1 3/2	2.00	1871,0621	1871,0603	0,0018
2	1	P1 5/2	2.00	1867,6678	1867,6650	0,0028
3	1	P1 7/2	2.00	1864,2372	1864,2355	0,0017
4	1	P1 9/2	2.00	1860,7738	1860,7719	0,0019
5	1	P1 11/2	2.00	1857,2751	1857,2742	0,0009
6	1	P1 13/2	2.00	1853,7426	1853,7423	0,0003
7	1	P1 15/2	2.00	1850,1777	1850,1763	0,0014
8	1	P1 17/2	2.00	1846,5784	1846,5762	0,0022
9	1	P1 19/2	2.00	1842,9420	1842,9420	0,0000
10	1	P1 21/2	2.00	1839,2729	1839,2736	-0,0007
11	1	P1 23/2	2.00	1835,5705	1835,5712	-0,0007
12	1	P1 25/2	2.00	1831,8345	1831,8346	-0,0001
13	1	P1 27/2	2.00	1828,0622	1828,0640	-0,0018
14	1	P1 29/2	2.00	1824,2581	1824,2593	-0,0012
15	1	P1 31/2	2.00	1820,4175	1820,4206	-0,0031
16	1	P1 33/2	2.00	1816,5447	1816,5479	-0,0032
17	1	P1 35/2	2.00	1812,6403	1812,6412	-0,0009
18	1	P1 37/2	2.00	1808,6959	1808,7007	-0,0048
19	1	P1 39/2	3.00	1804,7237	1804,7264	-0,0027
20	1	P1 41/2	2.00	1800,7203	1800,7183	0,0020
21	1	P1 43/2	0.00	1796,6884	1796,6767	0,0117
22	1	P1 45/2	0.00	1792,6158	1792,6016	0,0142
23	1	P1 47/2	1.00	1788,4977	1788,4931	0,0046
24	1	P1 49/2	1.25	1784,3583	1784,3515	0,0068
25	1	P1 51/2	1.25	1780,1857	1780,1769	0,0088
26	1	P1 53/2	1.25	1775,9811	1775,9695	0,0116
27	1	P1 55/2	1.06	1771,7412	1771,7296	0,0116
28	1	P1 57/2	1.00	1767,4719	1767,4575	0,0144
29	1	P1 59/2	1.00	1763,1680	1763,1535	0,0145
30	1	P1 61/2	1.00	1758,8344	1758,8179	0,0165
31	1	P1 63/2	0,31	1754,4648	1754,4511	0,0137
32	1	P1 67/2	0.00	1745,6376	1745,6256	0,0120
33	1	P1 69/2	0,25	1741,1611	1741,1678	-0,0067
34	1	P1 71/2	0,31	1736,6771	1736,6808	-0,0037
35	1	P1 73/2	0,80	1732,1552	1732,1651	-0,0099
36	1	P1 75/2	0,50	1727,5964	1727,6214	-0,0250



37	1	P2	5/2	1.25	1867.2154	1867,2148	0,0006
38	1	P2	7/2	2.00	1863.6850	1863,6853	=0,0003
39	1	P2	9/2	2.00	1860.1206	1860,1206	0,0000
40	1	P2	11/2	2.00	1856.5204	1856,5209	=0,0005
41	1	P2	13/2	2.00	1852.8884	1852,8864	0,0020
42	1	P2	15/2	2.00	1849.2157	1849,2175	=0,0018
43	1	P2	17/2	2.00	1845.5164	1845,5143	0,0021
44	1	P2	19/2	2.00	1841.7786	1841,7772	0,0014
45	1	P2	21/2	2.00	1838.0078	1838,0064	0,0014
46	1	P2	23/2	2.00	1834.2044	1834,2021	0,0023
47	1	P2	25/2	2.00	1830.3675	1830,3645	0,0030
48	1	P2	27/2	2.00	1826.4956	1826,4940	0,0016
49	1	P2	29/2	2.00	1822.5922	1822,5907	0,0015
50	1	P2	31/2	2.00	1818.6562	1818,6549	0,0013
51	1	P2	33/2	2.00	1814.6895	1814,6868	0,0027
52	1	P2	35/2	0.00	1810.6848	1810,6866	=0,0018
53	1	P2	37/2	2.00	1806.6560	1806,6544	0,0016
54	1	P2	39/2	4.00	1802.5904	1802,5905	=0,0001
55	1	P2	41/2	2.00	1798.4906	1798,4950	=0,0044
56	1	P2	43/2	2.00	1794.3653	1794,3681	=0,0028
57	1	P2	45/2	1.25	1790.2101	1790,2098	0,0003
58	1	P2	47/2	2.00	1786.0183	1786,0202	=0,0019
59	1	P2	49/2	0.50	1781.7936	1781,7996	=0,0060
60	1	P2	51/2	1.25	1777.5433	1777,5478	=0,0045
61	1	P2	53/2	1.06	1773.2571	1773,2649	=0,0078
62	1	P2	55/2	1.00	1768.9423	1768,9510	=0,0087
63	1	P2	57/2	1.00	1764.5973	1764,6060	=0,0087
64	1	P2	59/2	1.00	1760.2179	1760,2298	=0,0119
65	1	P2	63/2	0.00	1751.3985	1751,3834	0,0151
66	1	P2	65/2	0.25	1746.9073	1746,9129	=0,0056
67	1	P2	67/2	0.25	1742.4046	1742,4106	=0,0060
68	1	P2	69/2	0.25	1737.8741	1737,8762	=0,0021
69	1	P2	71/2	0.00	1733.3576	1733,3094	0,0482
70	1	P2	73/2	0.87	1728.7216	1728,7099	0,0117
71	1	R1	1/2	2.00	1881.0430	1881,0413	0,0017
72	1	R1	3/2	0.12	1884.3080	1884,2999	0,0081
73	1	R1	5/2	2.00	1887.5249	1887,5242	0,0007
74	1	R1	7/2	2.00	1890.7149	1890,7142	0,0007
75	1	R1	9/2	2.00	1893.8708	1893,8698	0,0010
76	1	R1	11/2	2.00	1896.9927	1896,9911	0,0016
77	1	R1	13/2	2.00	1900.0795	1900,0778	0,0017
78	1	R1	15/2	2.00	1903.1310	1903,1301	0,0009
79	1	R1	17/2	4.00	1906.1482	1906,1476	0,0006
80	1	R1	19/2	3.00	1909.1314	1909,1305	0,0009
81	1	R1	21/2	3.00	1912.0785	1912,0785	=0,0000
82	1	R1	23/2	3.00	1914.9911	1914,9916	=0,0005
83	1	R1	25/2	2.00	1917.8670	1917,8697	=0,0027
84	1	R1	27/2	2.00	1920.7128	1920,7126	0,0002
85	1	R1	29/2	2.00	1923.5204	1923,5202	0,0002
86	1	R1	31/2	2.00	1926.2911	1926,2923	=0,0012
87	1	R1	33/2	2.00	1929.0276	1929,0288	=0,0012
88	1	R1	35/2	2.00	1931.7289	1931,7296	=0,0007
89	1	R1	37/2	2.00	1934.3935	1934,3944	=0,0009
90	1	R1	39/2	2.00	1937.0224	1937,0232	=0,0008



91	1	R1	41/2	2.00	1939,6158	1939,6156	0,0002
92	1	R1	43/2	2.00	1942,1686	1942,1716	-0,0030
93	1	R1	45/2	2.00	1944,6914	1944,6910	0,0004
94	1	R1	47/2	2.00	1947,1705	1947,1734	-0,0029
95	1	R1	49/2	1.00	1949,6218	1949,6189	0,0029
96	1	R1	51/2	2.00	1952,0242	1952,0270	-0,0028
97	1	R1	53/2	2.00	1954,3920	1954,3977	-0,0057
98	1	R1	55/2	2.00	1956,7264	1956,7306	-0,0042
99	1	R1	57/2	2.00	1959,0258	1959,0257	0,0001
100	1	R1	59/2	2.00	1961,2817	1961,2827	-0,0010
101	1	R1	63/2	2.00	1965,6779	1965,6815	-0,0036
102	1	R1	65/2	3.00	1967,8200	1967,8228	-0,0028
103	1	R1	67/2	2.00	1969,9236	1969,9253	-0,0017
104	1	R1	69/2	0.00	1971,9874	1971,9886	-0,0012
105	1	R1	71/2	4.25	1974,0119	1974,0125	-0,0006
106	1	R1	73/2	4.06	1975,9970	1975,9970	-0,0000
107	1	R1	77/2	3.27	1979,8486	1979,8467	0,0019
108	1	R1	79/2	1.02	1981,7183	1981,7117	0,0066
109	1	R1	81/2	0.25	1983,5390	1983,5365	0,0025
110	1	R1	83/2	0.03	1985,3251	1985,3211	0,0040
111	1	R2	5/2	0.50	1887,6334	1887,6378	-0,0044
112	1	R2	7/2	2.00	1890,9134	1890,9138	-0,0004
113	1	R2	9/2	2.00	1894,1523	1894,1526	-0,0003
114	1	R2	11/2	2.00	1897,3539	1897,3541	-0,0002
115	1	R2	13/2	2.00	1900,5179	1900,5180	-0,0001
116	1	R2	15/2	2.00	1903,6422	1903,6442	-0,0020
117	1	R2	17/2	4.00	1906,7335	1906,7325	0,0010
118	1	R2	19/2	3.00	1909,7827	1909,7827	0,0000
119	1	R2	21/2	3.00	1912,7972	1912,7946	0,0026
120	1	R2	23/2	2.00	1915,7691	1915,7680	0,0011
121	1	R2	25/2	2.00	1918,7034	1918,7029	0,0005
122	1	R2	27/2	2.00	1921,5985	1921,5990	-0,0005
123	1	R2	29/2	2.00	1924,4551	1924,4563	-0,0012
124	1	R2	31/2	2.00	1927,2751	1927,2745	0,0006
125	1	R2	33/2	2.00	1930,0551	1930,0536	0,0015
126	1	R2	35/2	2.00	1932,7929	1932,7935	-0,0006
127	1	R2	37/2	2.00	1935,4916	1935,4940	-0,0024
128	1	R2	39/2	2.00	1938,1563	1938,1550	0,0013
129	1	R2	41/2	2.00	1940,7772	1940,7765	0,0007
130	1	R2	43/2	2.00	1943,3607	1943,3583	0,0024
131	1	R2	45/2	2.00	1945,9001	1945,9004	-0,0003
132	1	R2	47/2	1.00	1948,4071	1948,4027	0,0044
133	1	R2	49/2	1.00	1950,8699	1950,8651	0,0048
134	1	R2	51/2	2.00	1953,2875	1953,2875	0,0000
135	1	R2	53/2	2.00	1955,6704	1955,6698	0,0006
136	1	R2	55/2	2.00	1958,0141	1958,0121	0,0020
137	1	R2	57/2	2.00	1960,3188	1960,3141	0,0047
138	1	R2	59/2	2.00	1962,5791	1962,5759	0,0032
139	1	R2	61/2	2.00	1964,8004	1964,7974	0,0030
140	1	R2	63/2	3.00	1966,9819	1966,9784	0,0035
141	1	R2	67/2	5.00	1971,2184	1971,2190	-0,0006
142	1	R2	69/2	4.25	1973,2801	1973,2783	0,0018
143	1	R2	71/2	4.06	1975,2977	1975,2968	0,0009
144	1	R2	73/2	4.06	1977,2728	1977,2745	-0,0017



145	1	R2	75/2	2.52	1979,2082	1979,2112	=0,0030
146	1	R2	79/2	0.25	1982,9551	1982,9610	=0,0059
147	1	R2	81/2	0.03	1984,7701	1984,7739	=0,0038
148	1	PH	5/2	3.50	1987,3424	1987,3497	=0,0073
149	1	PH	7/2	4.25	1984,1496	1984,1554	=0,0058
150	1	PH	13/2	0.81	1974,9266	1974,9249	0,0017
151	1	PH	19/2	0.59	1966,2034	1966,2010	0,0024
152	1	PH	21/2	0.00	1963,3488	1963,3990	=0,0502
153	1	PH	23/2	0.83	1960,6465	1960,6472	=0,0007
154	1	PH	27/2	0.22	1955,2907	1955,2855	0,0052
155	1	PH	29/2	0.50	1952,6705	1952,6714	=0,0009
156	1	PH	31/2	0.19	1950,0931	1950,0986	=0,0055
157	1	QH	3/2	3.44	1995,7093	1995,7098	=0,0005
158	1	QH	5/2	3.44	1995,8561	1995,8596	=0,0035
159	1	QH	7/2	5.75	1996,0692	1996,0685	0,0007
160	1	QH	9/2	5.75	1996,3367	1996,3358	0,0009
161	1	QH	11/2	6.50	1996,6594	1996,6605	=0,0011
162	1	QH	13/2	4.25	1997,0403	1997,0414	=0,0011
163	1	QH	15/2	6.25	1997,4819	1997,4773	0,0046
164	1	QH	17/2	7.25	1997,9706	1997,9666	0,0040
165	1	QH	19/2	7.25	1998,5101	1998,5074	0,0027
166	1	QH	21/2	5.25	1999,1019	1999,0981	0,0038
167	1	QH	23/2	7.25	1999,7395	1999,7364	0,0031
168	1	QH	25/2	6.71	2000,4216	2000,4202	0,0014
169	1	QH	27/2	5.71	2001,1481	2001,1471	0,0010
170	1	QH	29/2	6.25	2001,9131	2001,9148	=0,0017
171	1	QH	31/2	6.25	2002,7202	2002,7207	=0,0005
172	1	QH	33/2	6.52	2003,5586	2003,5621	=0,0035
173	1	QH	35/2	0.06	2004,4293	2004,4364	=0,0071
174	1	QH	37/2	5.47	2005,3351	2005,3409	=0,0058
175	1	QH	39/2	2.02	2006,2678	2006,2728	=0,0050
176	1	QH	41/2	0.75	2007,2268	2007,2293	=0,0025
177	1	QH	43/2	0.37	2008,2061	2008,2077	=0,0016
178	1	QH	45/2	0.12	2009,2108	2009,2055	0,0053
179	1	QH	47/2	0.02	2010,2235	2010,2198	0,0037
180	1	RH	1/2	6.25	2000,7202	2000,7259	=0,0057
181	1	RH	3/2	4.06	2004,2184	2004,2197	=0,0013
182	1	RH	5/2	5.25	2007,7710	2007,7726	=0,0016
183	1	RH	7/2	6.25	2011,3816	2011,3838	=0,0022
184	1	RH	9/2	3.25	2015,0516	2015,0524	=0,0008
185	1	RH	11/2	2.25	2018,7790	2018,7770	0,0020
186	1	RH	13/2	2.25	2022,5563	2022,5565	=0,0002
187	1	RH	15/2	2.25	2026,3944	2026,3890	0,0054
188	1	RH	17/2	2.25	2030,2763	2030,2730	0,0033
189	1	RH	19/2	2.25	2034,2086	2034,2065	0,0021
190	1	RH	21/2	2.25	2038,1911	2038,1873	0,0038
191	1	RH	23/2	2.25	2042,2159	2042,2132	0,0027
192	1	RH	25/2	1.25	2046,2841	2046,2818	0,0023
193	1	RH	27/2	2.06	2050,3927	2050,3905	0,0022
194	1	RH	29/2	2.02	2054,5361	2054,5369	=0,0008
195	1	RH	31/2	2.02	2058,7180	2058,7181	=0,0001
196	1	RH	33/2	0.50	2062,9301	2062,9314	=0,0013
197	1	RH	35/2	0.31	2067,1735	2067,1740	=0,0005
198	1	RH	37/2	0.12	2071,4369	2071,4429	=0,0060

199	1	RH	39/2	0.12	2075.7358	2075.7353	0.0005
200	1	RH	41/2	0.00	2080.0497	2080.0483	0.0014
201	1	PL	7/2	0.02	1743.7736	1743.7655	0.0081
202	1	PL	9/2	0.00	1739.8602	1739.8721	-0.0119
203	1	PL	11/2	0.33	1735.8506	1735.8512	-0.0006
204	1	PL	13/2	0.14	1731.7099	1731.7039	0.0060
205	1	PL	15/2	0.45	1727.4296	1727.4315	-0.0019
206	1	PL	17/2	0.00	1723.0406	1723.0357	0.0049
207	1	PL	19/2	0.00	1718.5314	1718.5182	0.0132
208	1	PL	21/2	0.89	1713.8731	1713.8810	-0.0079
209	1	PL	23/2	2.35	1709.1216	1709.1261	-0.0045
210	1	PL	25/2	0.41	1704.2579	1704.2558	0.0021
211	1	PL	29/2	0.31	1694.1797	1694.1787	0.0010
212	1	PL	31/2	0.06	1688.9736	1688.9770	-0.0034
213	1	PL	33/2	0.31	1683.6705	1683.6701	0.0004
214	1	PL	35/2	0.06	1678.2606	1678.2608	-0.0002
215	1	QL	3/2	0.00	1756.1344	1756.1304	0.0040
216	1	QL	7/2	0.37	1755.3554	1755.3499	0.0055
217	1	QL	9/2	0.00	1754.7463	1754.7663	-0.0200
218	1	QL	13/2	0.16	1753.2180	1753.2170	0.0010
219	1	QL	15/2	0.00	1752.2486	1752.2539	-0.0053
220	1	QL	17/2	0.00	1751.1800	1751.1670	0.0130
221	1	QL	21/2	0.00	1748.6199	1748.6294	-0.0095
222	1	QL	23/2	0.00	1747.1732	1747.1825	-0.0093
223	1	RL	7/2	0.00	1770.2551	1770.2441	0.0110
224	1	RL	17/2	2.08	1782.6006	1782.6071	-0.0065
225	1	RL	21/2	0.18	1786.6781	1786.6858	-0.0077
226	1	RL	27/2	0.04	1791.9257	1791.9211	0.0046
227	1	RL	29/2	0.04	1793.4459	1793.4395	0.0064

S.D. = 0.0035



APPENDIX IX-B

FREQUENCY FIT FOR 15N16O

N	V	LINE	WGT,	OBSERVED	PREDICTED	(O-P)
1	1	P1 77/2	0.50	1695,7322	1695,7387	-0,0065
2	1	P1 75/2	0.12	1700,1321	1700,1400	-0,0079
3	1	P1 73/2	0.00	1704,4740	1704,5128	-0,0388
4	1	P1 71/2	4.00	1708,8576	1708,8568	0,0008
5	1	P1 67/2	0.00	1717,4356	1717,4576	-0,0220
6	1	P1 65/2	0.00	1721,7132	1721,7138	-0,0006
7	1	P1 63/2	1.00	1725,9500	1725,9403	0,0097
8	1	P1 61/2	0.00	1730,1360	1730,1367	-0,0007
9	1	P1 59/2	0.00	1734,3142	1734,3029	0,0113
10	1	P1 57/2	1.06	1738,4392	1738,4388	0,0004
11	1	P1 55/2	1.06	1742,5464	1742,5440	0,0024
12	1	P1 53/2	1.06	1746,6172	1746,6185	-0,0013
13	1	P1 51/2	0.31	1750,6611	1750,6621	-0,0010
14	1	P1 49/2	0.50	1754,6751	1754,6747	0,0004
15	1	P1 47/2	0.00	1758,6554	1758,6560	-0,0006
16	1	P1 45/2	1.00	1762,6093	1762,6061	0,0032
17	1	P1 43/2	1.06	1766,5163	1766,5247	-0,0084
18	1	P1 41/2	1.25	1770,4089	1770,4118	-0,0029
19	1	P1 39/2	2.00	1774,2697	1774,2672	0,0025
20	1	P1 37/2	2.00	1778,0889	1778,0909	-0,0020
21	1	P1 35/2	2.00	1781,8808	1781,8829	-0,0021
22	1	P1 33/2	2.00	1785,6504	1785,6429	0,0075
23	1	P1 31/2	2.00	1789,3694	1789,3710	-0,0016
24	1	P1 29/2	2.00	1793,0696	1793,0671	0,0025
25	1	P1 27/2	2.00	1796,7309	1796,7311	-0,0002
26	1	P1 25/2	2.00	1800,3657	1800,3631	0,0026
27	1	P1 23/2	2.00	1803,9610	1803,9628	-0,0018
28	1	P1 21/2	2.00	1807,5305	1807,5304	0,0001
29	1	P1 19/2	2.00	1811,0696	1811,0657	0,0039
30	1	P1 17/2	2.00	1814,5759	1814,5688	0,0071
31	1	P1 15/2	2.00	1818,0386	1818,0396	-0,0010
32	1	P1 13/2	2.00	1821,4766	1821,4780	-0,0014
33	1	P1 11/2	2.00	1824,8814	1824,8841	-0,0027
34	1	P1 9/2	2.00	1828,2559	1828,2578	-0,0019
35	1	P1 7/2	2.00	1831,5973	1831,5991	-0,0018
36	1	P1 5/2	2.00	1834,9074	1834,9080	-0,0006

1. 2.

3.

4.

5.

6.

7.

8.

9.

10.

11.

12.

13.

14.

15.

16.

17.

18.

19.

20.

21.

22.

23.

24.

25.

26.

27.

28.

29.

30.

31.

32.

33.

34.

35.

36.

37.

38.

39.

40.

41.

42.

43.

44.

45.

46.

47.

48.

37	1	P1	3/2	2.00	1838,1834	1838,1844	=0,0010
38	1	R1	1/2	2.00	1847,8135	1847,8187	=0,0052
39	1	R1	5/2	0.50	1854,0782	1854,0787	=0,0005
40	1	R1	7/2	2.00	1857,1583	1857,1598	=0,0015
41	1	R1	9/2	0.50	1860,2025	1860,2082	=0,0057
42	1	R1	11/2	2.00	1863,2221	1863,2238	=0,0017
43	1	R1	13/2	2.00	1866,2067	1866,2068	=0,0001
44	1	R1	15/2	2.00	1869,1583	1869,1568	0,0015
45	1	R1	17/2	2.00	1872,0747	1872,0740	0,0007
46	1	R1	19/2	2.00	1874,9630	1874,9583	0,0047
47	1	R1	21/2	2.00	1877,8083	1877,8095	=0,0012
48	1	R1	23/2	2.00	1880,6324	1880,6276	0,0048
49	1	R1	25/2	2.00	1883,4177	1883,4125	0,0052
50	1	R1	27/2	2.00	1886,1654	1886,1641	0,0013
51	1	R1	29/2	3.00	1888,8816	1888,8823	=0,0007
52	1	R1	31/2	1.00	1891,5711	1891,5670	0,0041
53	1	R1	33/2	0.50	1894,2169	1894,2181	=0,0012
54	1	R1	35/2	2.00	1896,8374	1896,8354	0,0020
55	1	R1	37/2	2.00	1899,4234	1899,4187	0,0047
56	1	R1	39/2	2.00	1901,9697	1901,9681	0,0016
57	1	R1	41/2	2.00	1904,4862	1904,4831	0,0031
58	1	R1	43/2	2.00	1906,9634	1906,9638	=0,0004
59	1	R1	45/2	2.00	1909,4106	1909,4098	0,0008
60	1	R1	47/2	2.00	1911,8191	1911,8211	=0,0020
61	1	R1	49/2	2.00	1914,1965	1914,1972	=0,0007
62	1	R1	51/2	1.00	1916,5342	1916,5382	=0,0040
63	1	R1	53/2	2.00	1918,8406	1918,8436	=0,0030
64	1	R1	55/2	2.00	1921,1077	1921,1132	=0,0055
65	1	R1	57/2	1.00	1923,3434	1923,3468	=0,0034
66	1	R1	59/2	2.00	1925,5398	1925,5440	=0,0042
67	1	R1	61/2	2.00	1927,7002	1927,7045	=0,0043
68	1	R1	63/2	2.00	1929,8260	1929,8280	=0,0020
69	1	R1	65/2	2.00	1931,9140	1931,9142	=0,0002
70	1	R1	67/2	1.25	1933,9656	1933,9627	0,0029
71	1	R1	69/2	1.25	1935,9802	1935,9731	0,0071
72	1	R1	71/2	0.50	1937,9557	1937,9450	0,0107
73	1	R1	75/2	0.00	1941,8065	1941,7716	0,0349
74	1	P2	75/2	0.12	1696,8332	1696,8213	0,0119
75	1	P2	73/2	0.50	1701,2654	1701,2611	0,0043
76	1	P2	71/2	0.50	1705,6775	1705,6716	0,0059
77	1	P2	67/2	0.00	1714,4074	1714,4051	0,0023
78	1	P2	65/2	0.00	1718,7343	1718,7282	0,0061
79	1	P2	63/2	0.19	1723,0202	1723,0221	=0,0019
80	1	P2	61/2	1.37	1727,2815	1727,2869	=0,0054
81	1	P2	59/2	1.06	1731,5179	1731,5226	=0,0047
82	1	P2	57/2	0,31	1735,7232	1735,7290	=0,0058
83	1	P2	55/2	0.00	1739,8789	1739,9062	=0,0273
84	1	P2	53/2	1.06	1744,0501	1744,0541	=0,0040
85	1	P2	51/2	0.31	1748,1706	1748,1726	=0,0020
86	1	P2	49/2	0.50	1752,2571	1752,2617	=0,0046
87	1	P2	47/2	1.06	1756,3202	1756,3212	=0,0010
88	1	P2	45/2	0.25	1760,3483	1760,3510	=0,0027
89	1	P2	43/2	1.00	1764,3489	1764,3510	=0,0021
90	1	P2	41/2	1.25	1768,3187	1768,3210	=0,0023

91	1	P2	39/2	1.25	1772,2598	1772,2610	-0,0012
92	1	P2	37/2	2.00	1776,1782	1776,1708	0,0074
93	1	P2	35/2	2.00	1780,0440	1780,0503	-0,0063
94	1	P2	33/2	2.00	1783,8990	1783,8992	-0,0002
95	1	P2	31/2	2.00	1787,7169	1787,7174	-0,0005
96	1	P2	29/2	2.00	1791,5102	1791,5047	0,0055
97	1	P2	27/2	2.00	1795,2653	1795,2610	0,0043
98	1	P2	25/2	2.00	1798,9888	1798,9860	0,0028
99	1	P2	23/2	0.50	1802,6814	1802,6796	0,0018
100	1	P2	21/2	2.00	1806,3468	1806,3415	0,0053
101	1	P2	19/2	2.00	1809,9735	1809,9716	0,0019
102	1	P2	17/2	2.00	1813,5698	1813,5697	0,0001
103	1	P2	15/2	2.00	1817,1362	1817,1355	0,0007
104	1	P2	13/2	2.00	1820,6702	1820,6688	0,0014
105	1	P2	11/2	0.00	1824,1794	1824,1694	0,0100
106	1	P2	9/2	2.00	1827,6382	1827,6372	0,0010
107	1	P2	7/2	2.00	1831,0739	1831,0718	0,0021
108	1	P2	5/2	2.00	1834,4720	1834,4731	-0,0011
109	1	R2	5/2	0.00	1854,1636	1854,1687	-0,0051
110	1	R2	7/2	0.00	1857,3063	1857,3306	-0,0243
111	1	R2	9/2	2.00	1860,4573	1860,4575	-0,0002
112	1	R2	11/2	2.00	1863,5501	1863,5491	0,0010
113	1	R2	13/2	2.00	1866,6047	1866,6053	-0,0006
114	1	R2	15/2	2.00	1869,6253	1869,6258	-0,0005
115	1	R2	17/2	2.00	1872,6106	1872,6105	0,0001
116	1	R2	19/2	2.00	1875,5649	1875,5592	0,0057
117	1	R2	21/2	2.00	1878,4693	1878,4718	-0,0025
118	1	R2	23/2	2.00	1881,3466	1881,3480	-0,0014
119	1	R2	25/2	2.00	1884,1852	1884,1876	-0,0024
120	1	R2	27/2	4.00	1886,9869	1886,9907	-0,0038
121	1	R2	29/2	3.00	1889,7524	1889,7569	-0,0045
122	1	R2	31/2	1.00	1892,4833	1892,4862	-0,0029
123	1	R2	33/2	2.00	1895,1834	1895,1784	0,0050
124	1	R2	35/2	2.00	1897,8304	1897,8334	-0,0030
125	1	R2	37/2	0.31	1900,4495	1900,4511	-0,0016
126	1	R2	39/2	0.50	1903,0334	1903,0314	0,0020
127	1	R2	41/2	2.00	1905,5724	1905,5743	-0,0019
128	1	R2	43/2	2.00	1908,0801	1908,0796	0,0005
129	1	R2	45/2	2.00	1910,5469	1910,5473	-0,0004
130	1	R2	47/2	2.00	1912,9780	1912,9773	0,0007
131	1	R2	49/2	2.00	1915,3715	1915,3697	0,0018
132	1	R2	51/2	2.00	1917,7274	1917,7243	0,0031
133	1	R2	53/2	2.00	1920,0435	1920,0412	0,0023
134	1	R2	55/2	2.00	1922,3288	1922,3204	0,0084
135	1	R2	57/2	0.50	1924,5620	1924,5619	0,0001
136	1	R2	59/2	1.00	1926,7715	1926,7657	0,0058
137	1	R2	63/2	2.00	1931,0602	1931,0607	-0,0005
138	1	R2	65/2	1.25	1933,1533	1933,1520	0,0013
139	1	R2	67/2	1.25	1935,1993	1935,2060	-0,0067
140	1	R2	71/2	0.12	1939,1749	1939,2024	-0,0275
141	1	PL	29/2	0.06	1663,5706	1663,5676	0,0030
142	1	PL	25/2	0.25	1673,1964	1673,2011	-0,0047
143	1	PL	23/2	0.33	1677,8582	1677,8589	-0,0007
144	1	PL	21/2	0.31	1682,4009	1682,4079	-0,0070

145	1	PL	19/2	0.50	1686,8447	1686,8461	-0,0014
146	1	PL	17/2	0.25	1691,1701	1691,1717	-0,0016
147	1	PL	15/2	0.00	1695,4485	1695,3830	0,0655
148	1	PL	13/2	0.00	1699,4708	1699,4785	-0,0077
149	1	PL	11/2	2.00	1703,4600	1703,4569	0,0031
150	1	PL	9/2	0.00	1707,3133	1707,3169	-0,0036
151	1	PL	7/2	2.00	1711,0583	1711,0574	0,0009
152	1	PL	3/2	0.00	1718,1864	1718,1770	0,0094
153	1	QL	31/2	0.50	1708,0992	1708,0993	-0,0001
154	1	QL	27/2	0.00	1711,5478	1711,5574	-0,0096
155	1	QL	21/2	2.00	1715,9443	1715,9509	-0,0066
156	1	QL	19/2	0.50	1717,1929	1717,1956	-0,0027
157	1	QL	17/2	0.00	1718,3249	1718,3274	-0,0025
158	1	QL	15/2	2.00	1719,3415	1719,3446	-0,0031
159	1	QL	13/2	2.00	1720,2422	1720,2457	-0,0035
160	1	QL	7/2	2.00	1722,2386	1722,2403	-0,0017
161	1	QL	5/2	2.00	1722,6680	1722,6655	0,0025
162	1	RL	7/2	0.00	1736,6579	1736,6181	0,0398
163	1	RL	27/2	0.06	1757,8669	1757,8696	-0,0027
164	1	PH	21/2	0.04	1931,4675	1931,4640	0,0035
165	1	PH	19/2	0.00	1934,2000	1934,1913	0,0087
166	1	PH	15/2	0.00	1939,8185	1939,7920	0,0265
167	1	PH	13/2	0.50	1942,6763	1942,6683	0,0080
168	1	PH	11/2	0.00	1945,5907	1945,5967	-0,0060
169	1	PH	9/2	0.52	1948,5692	1948,5781	-0,0089
170	1	PH	7/2	1.50	1951,6154	1951,6135	0,0019
171	1	PH	5/2	0.52	1954,7006	1954,7034	-0,0028
172	1	QH	3/2	1.00	1962,7679	1962,7726	-0,0047
173	1	QH	5/2	4.00	1962,9055	1962,9102	-0,0047
174	1	QH	7/2	4.00	1963,0996	1963,1023	-0,0027
175	1	QH	9/2	4.00	1963,3476	1963,3481	-0,0005
176	1	QH	11/2	4.00	1963,6441	1963,6469	-0,0028
177	1	QH	13/2	5.00	1963,9958	1963,9977	-0,0019
178	1	QH	15/2	3.06	1964,4011	1964,3991	0,0020
179	1	QH	17/2	1.19	1964,8510	1964,8501	0,0009
180	1	QH	19/2	3.00	1965,3521	1965,3489	0,0032
181	1	QH	21/2	4.00	1965,8982	1965,8941	0,0041
182	1	QH	23/2	4.00	1966,4860	1966,4837	0,0023
183	1	QH	25/2	1.60	1967,1174	1967,1161	0,0013
184	1	QH	27/2	0.47	1967,7831	1967,7890	-0,0059
185	1	QH	29/2	4.00	1968,5015	1968,5004	0,0011
186	1	QH	31/2	4.00	1969,2411	1969,2481	-0,0070
187	1	QH	33/2	2.00	1970,0260	1970,0298	-0,0038
188	1	QH	37/2	0.50	1971,6784	1971,6858	-0,0074
189	1	QH	39/2	0.12	1972,5484	1972,5553	-0,0069
190	1	QH	41/2	0.03	1973,4387	1973,4492	-0,0105
191	1	RH	1/2	1.00	1967,6108	1967,6141	-0,0033
192	1	RH	7/2	2.00	1977,8723	1977,8723	-0,0000
193	1	RH	9/2	2.00	1981,4000	1981,3984	0,0016
194	1	RH	11/2	2.00	1984,9774	1984,9763	0,0011
195	1	RH	13/2	2.00	1988,6050	1988,6047	0,0003
196	1	RH	15/2	2.00	1992,2837	1992,2824	0,0013
197	1	RH	17/2	2.00	1996,0100	1996,0077	0,0023
198	1	RH	19/2	2.00	1999,7806	1999,7789	0,0017

5. The fifth part of the document concludes by emphasizing the importance of the accounting department in the overall success of the organization. It states that accurate financial reporting is essential for making informed decisions and for ensuring the long-term sustainability of the business.



199	1	RH	21/2	2.00	2003.5978	2003,5943	0,0035
200	1	RH	23/2	2.00	2007.4539	2007,4519	0,0020
201	1	RH	25/2	1.54	2011.3507	2011,3496	0,0011
202	1	RH	27/2	2.00	2015.2872	2015,2852	0,0020
203	1	RH	29/2	0.50	2019.2551	2019,2564	0,0013
204	1	RH	31/2	0.12	2023.2536	2023,2609	0,0073
205	1	RH	33/2	0.02	2027.2882	2027,2962	0,0080
206	1	RH	35/2	0.02	2031.3528	2031,3599	0,0071
207	1	RH	37/2	0.00	2035.4363	2035,4494	0,0131

S.D. = 0,0035



APPENDIX X-A

FIT OF THE LAMBDA DOUBLET SPLITTINGS FOR 14N160

N	LINE	WGT.	OBS.	PRED.	(O-P)
1	PL 35/2	0.06	-0.1655	-0.1590	-0.0065
2	PL 33/2	0.31	-0.1639	-0.1556	-0.0083
3	PL 31/2	0.06	-0.1200	-0.1512	0.0312
4	PL 29/2	0.31	-0.1316	-0.1460	0.0144
5	PL 25/2	0.41	-0.1204	-0.1330	0.0126
6	PL 23/2	2.35	-0.1151	-0.1255	0.0104
7	PL 21/2	0.89	-0.1031	-0.1172	0.0141
8	PL 19/2	0.00	-0.1259	-0.1084	-0.0175
9	PL 17/2	0.00	-0.0771	-0.0991	0.0220
10	PL 15/2	0.33	-0.0677	-0.0893	0.0216
11	QL 23/2	0.00	-0.1545	-0.1403	-0.0142
12	QL 21/2	0.00	-0.1101	-0.1286	0.0185
13	QL 13/2	0.08	-0.0692	-0.0817	0.0125
14	RL 7/2	0.00	-0.0596	-0.0458	-0.0138
15	RL 17/2	0.00	-0.1045	-0.0968	-0.0077
16	RL 21/2	0.18	-0.1323	-0.1139	-0.0184
17	RL 27/2	0.04	-0.1365	-0.1345	-0.0020
18	RL 29/2	0.04	-0.1424	-0.1397	-0.0027
19	PH 31/2	0.19	0.1619	0.1514	0.0105
20	PH 29/2	0.50	0.1543	0.1461	0.0082
21	PH 27/2	0.22	0.1523	0.1400	0.0123
22	PH 23/2	0.83	0.1282	0.1255	0.0027
23	PH 19/2	0.59	0.1042	0.1085	-0.0043
24	QH 15/2	0.00	-0.0771	-0.0933	0.0162
25	QH 17/2	0.00	-0.0947	-0.1050	0.0103
26	QH 19/2	1.00	-0.1123	-0.1167	0.0044
27	QH 21/2	3.84	-0.1260	-0.1284	0.0024
28	QH 23/2	6.10	-0.1385	-0.1401	0.0016
29	QH 25/2	6.71	-0.1530	-0.1518	-0.0012
30	QH 27/2	5.71	-0.1626	-0.1636	0.0010
31	QH 29/2	6.25	-0.1765	-0.1753	-0.0012
32	QH 31/2	6.25	-0.1886	-0.1871	-0.0015
33	QH 33/2	6.52	-0.1995	-0.1988	-0.0007
34	QH 35/2	0.06	-0.2154	-0.2106	-0.0048
35	QH 37/2	5.47	-0.2229	-0.2224	-0.0005
36	QH 39/2	2.02	-0.2350	-0.2342	-0.0008

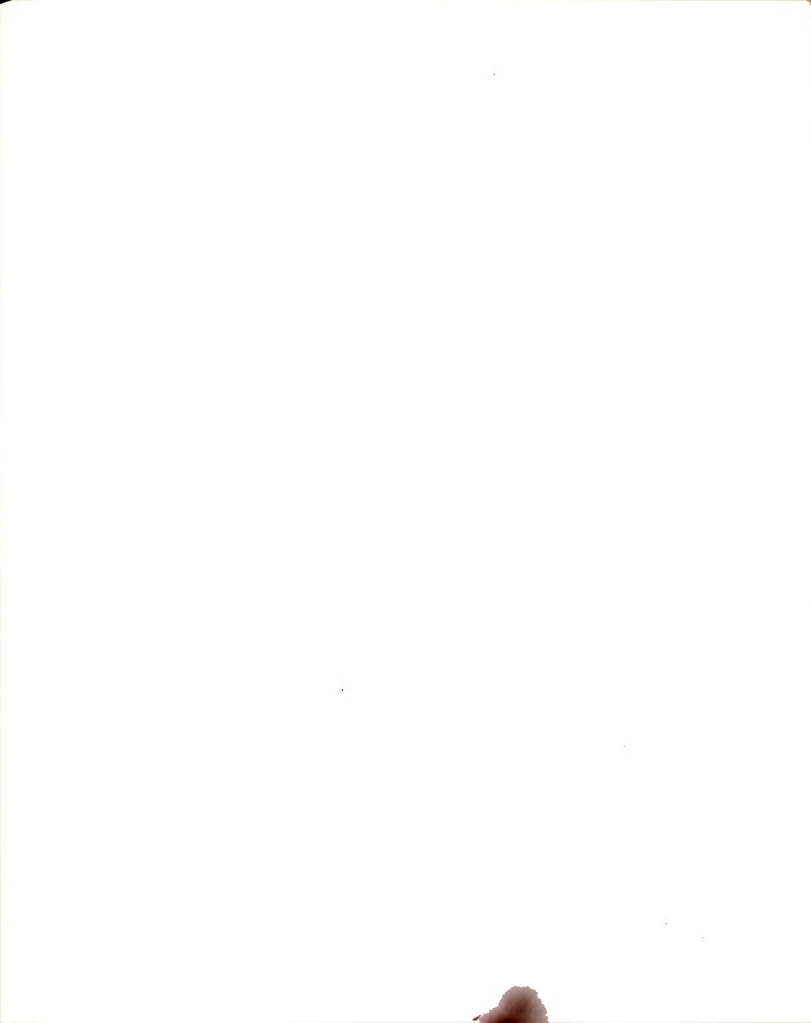


37	QH	41/2	0.75	-0.2520	-0.2460	-0.0060
38	QH	43/2	0.37	-0.2638	-0.2579	-0.0059
39	QH	45/2	0.12	-0.2726	-0.2698	-0.0028
40	QH	47/2	0.02	-0.2701	-0.2816	0.0115
41	RH	15/2	0.00	0.0651	0.0874	-0.0223
42	RH	17/2	0.00	0.0764	0.0968	-0.0204
43	RH	19/2	0.00	0.1016	0.1056	-0.0040
44	RH	21/2	0.25	0.1059	0.1138	-0.0079
45	RH	23/2	0.50	0.1170	0.1214	-0.0044
46	RH	27/2	2.06	0.1349	0.1343	0.0006
47	RH	29/2	2.02	0.1383	0.1396	-0.0013
48	RH	31/2	2.02	0.1476	0.1440	0.0036
49	RH	33/2	0.50	0.1479	0.1474	0.0005
50	RH	35/2	0.31	0.1544	0.1499	0.0045
51	RH	37/2	0.12	0.1542	0.1513	0.0029
52	RH	39/2	0.12	0.1595	0.1516	0.0079
53	RH	41/2	0.00	0.1789	0.1507	0.0282
54	P1	1/2	0.00	-0.0000	0.0117	-0.0117
55	P1	3/2	0.00	-0.0000	0.0117	-0.0117
56	P1	5/2	0.00	-0.0000	0.0118	-0.0118
57	P1	7/2	0.00	-0.0000	0.0120	-0.0120
58	P1	9/2	0.00	-0.0000	0.0125	-0.0125
59	P1	11/2	0.00	-0.0000	0.0132	-0.0132
60	P1	13/2	0.00	-0.0000	0.0142	-0.0142
61	P1	15/2	0.00	-0.0000	0.0156	-0.0156
62	P1	17/2	0.00	-0.0000	0.0173	-0.0173
63	P1	19/2	0.00	-0.0000	0.0196	-0.0196
64	P1	21/2	0.00	-0.0000	0.0224	-0.0224
65	P2	1/2	0.00	-0.0000	0.0000	-0.0000
66	P2	3/2	0.00	-0.0000	0.0000	-0.0000
67	P2	5/2	0.00	-0.0000	0.0001	-0.0001
68	P2	7/2	0.00	-0.0000	0.0002	-0.0002
69	P2	9/2	0.00	-0.0000	0.0003	-0.0003
70	P2	11/2	0.00	-0.0000	0.0004	-0.0004
71	P2	11/2	0.00	-0.0000	0.0004	-0.0004
72	P2	15/2	0.00	-0.0000	0.0008	-0.0008
73	P2	17/2	0.00	-0.0000	0.0011	-0.0011
74	P2	19/2	0.00	-0.0000	0.0014	-0.0014
75	P2	21/2	0.00	-0.0000	0.0017	-0.0017
76	R1	1/2	0.00	0.0000	-0.0116	0.0116
77	R1	3/2	0.00	0.0000	-0.0116	0.0116
78	R1	5/2	0.00	0.0000	-0.0115	0.0115
79	R1	7/2	0.00	0.0000	-0.0114	0.0114
80	R1	9/2	0.00	0.0000	-0.0112	0.0112
81	R1	11/2	0.00	0.0000	-0.0111	0.0111
82	R1	13/2	0.00	0.0000	-0.0109	0.0109
83	R1	15/2	0.00	0.0000	-0.0107	0.0107
84	R1	17/2	0.00	0.0000	-0.0105	0.0105
85	R1	19/2	0.00	0.0000	-0.0102	0.0102
86	R1	21/2	0.00	0.0000	-0.0099	0.0099
87	R2	1/2	0.00	0.0000	-0.0000	0.0000
88	R2	3/2	0.00	0.0000	-0.0001	0.0001
89	R2	5/2	0.00	0.0000	-0.0002	0.0002
90	R2	7/2	0.00	0.0000	-0.0003	0.0003



91	R2	9/2	0.00	0.0000	-0.0004	0.0004
92	R2	11/2	0.00	0.0000	-0.0006	0.0006
93	R2	13/2	0.00	0.0000	-0.0008	0.0008
94	R2	15/2	0.00	0.0000	-0.0010	0.0010
95	R2	17/2	0.00	0.0000	-0.0013	0.0013
96	R2	19/2	0.00	0.0000	-0.0015	0.0015
97	R2	21/2	0.00	0.0000	-0.0018	0.0018
98	Q1	1/2	0.00	0.0000	-0.0233	0.0233
99	Q1	3/2	0.00	0.0000	-0.0466	0.0466
100	Q1	5/2	0.00	0.0000	-0.0697	0.0697
101	Q1	7/2	0.00	0.0000	-0.0927	0.0927
102	Q1	9/2	0.00	0.0000	-0.1154	0.1154
103	Q1	11/2	0.00	0.0000	-0.1379	0.1379
104	Q1	13/2	0.00	0.0000	-0.1601	0.1601
105	Q1	15/2	0.00	0.0000	-0.1818	0.1818
106	Q1	17/2	0.00	0.0000	-0.2031	0.2031
107	Q1	19/2	0.00	0.0000	-0.2240	0.2240
108	Q1	21/2	0.00	0.0000	-0.2442	0.2442
109	Q1	23/2	0.00	0.0000	-0.2638	0.2638
110	Q1	25/2	0.00	0.0000	-0.2828	0.2828
111	Q1	27/2	0.00	0.0000	-0.3011	0.3011
112	Q1	29/2	0.00	0.0000	-0.3186	0.3186
113	Q1	31/2	0.00	0.0000	-0.3352	0.3352
114	Q2	3/2	0.00	0.0000	-0.0001	0.0001
115	Q2	5/2	0.00	0.0000	-0.0002	0.0002
116	Q2	7/2	0.00	0.0000	-0.0006	0.0006
117	Q2	9/2	0.00	0.0000	-0.0012	0.0012
118	Q2	11/2	0.00	0.0000	-0.0020	0.0020
119	Q2	13/2	0.00	0.0000	-0.0032	0.0032
120	Q2	15/2	0.00	0.0000	-0.0049	0.0049
121	Q2	17/2	0.00	0.0000	-0.0070	0.0070
122	Q2	19/2	0.00	0.0000	-0.0096	0.0096
123	Q2	21/2	0.00	0.0000	-0.0127	0.0127
124	Q2	23/2	0.00	0.0000	-0.0166	0.0166
125	Q2	25/2	0.00	0.0000	-0.0211	0.0211
126	Q2	27/2	0.00	0.0000	-0.0264	0.0264
127	Q2	29/2	0.00	0.0000	-0.0324	0.0324
128	Q2	31/2	0.00	0.0000	-0.0394	0.0394

S.D. = 0.0043



APPENDIX X-B

FIT OF THE LAMBDA DOUBLET SPLITTINGS FOR 15N160

N	LINE	WGT.	URS.	PRED.	(O-P)
1	PL 29/2	0.06	-0.1422	-0.1440	0.0018
2	PL 25/2	0.25	-0.1197	-0.1307	0.0110
3	PL 23/2	0.33	-0.1182	-0.1231	0.0049
4	QL 31/2	0.50	-0.1785	-0.1825	0.0040
5	QL 29/2	0.00	-0.2541	-0.1710	-0.0831
6	QL 27/2	0.00	-0.1465	-0.1595	0.0130
7	QL 25/2	0.00	-0.1227	-0.1480	0.0253
8	QL 21/2	2.00	-0.1296	-0.1251	-0.0045
9	QL 19/2	0.50	-0.1147	-0.1137	-0.0010
10	QL 17/2	0.00	-0.1042	-0.1023	-0.0019
11	QL 15/2	0.50	-0.0879	-0.0909	0.0030
12	RL 27/2	0.06	-0.1350	-0.1328	-0.0022
13	PH 21/2	0.04	0.1177	0.1149	0.0028
14	PH 19/2	0.00	0.1099	0.1061	0.0038
15	PH 15/2	0.00	0.1438	0.0872	0.0566
16	PH 13/2	0.00	0.0737	0.0771	-0.0034
17	QH 13/2	0.00	-0.0671	-0.0795	0.0124
18	QH 15/2	0.00	-0.0823	-0.0908	0.0085
19	QH 17/2	0.00	-0.0968	-0.1022	0.0054
20	QH 19/2	0.75	-0.1111	-0.1136	0.0025
21	QH 21/2	4.00	-0.1229	-0.1250	0.0021
22	QH 23/2	4.00	-0.1335	-0.1364	0.0029
23	QH 25/2	1.60	-0.1517	-0.1478	-0.0039
24	QH 27/2	0.47	-0.1556	-0.1592	0.0036
25	QH 29/2	4.00	-0.1713	-0.1706	-0.0007
26	QH 31/2	4.00	-0.1827	-0.1820	-0.0007
27	QH 33/2	2.00	-0.1963	-0.1935	-0.0028
28	QH 35/2	0.00	-0.2335	-0.2049	-0.0286
29	QH 37/2	0.50	-0.2160	-0.2164	0.0004
30	QH 39/2	0.12	-0.2273	-0.2279	0.0006
31	QH 41/2	0.03	-0.2425	-0.2394	-0.0031
32	RH 17/2	0.00	0.0909	0.0948	-0.0039
33	RH 19/2	0.50	0.1028	0.1035	-0.0007
34	RH 21/2	2.00	0.1117	0.1117	-0.0000
35	RH 23/2	2.00	0.1178	0.1194	-0.0016
36	RH 25/2	1.54	0.1225	0.1264	-0.0039

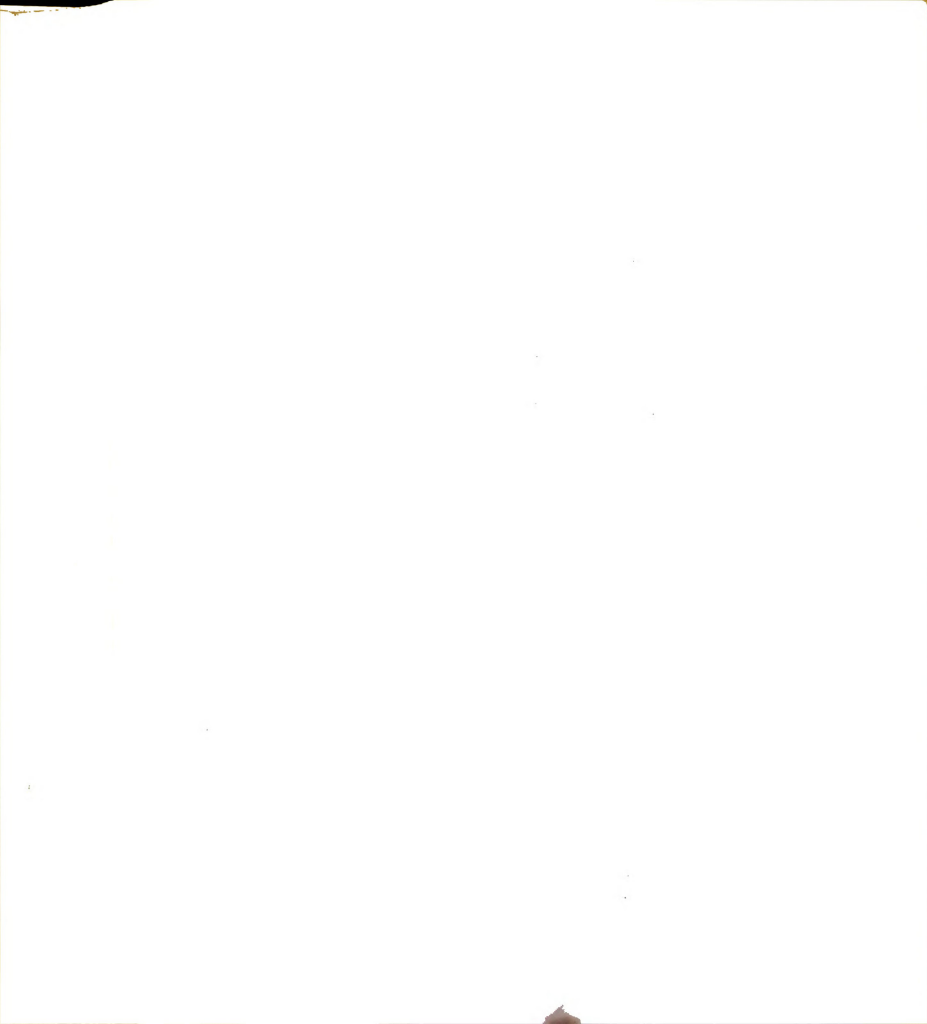


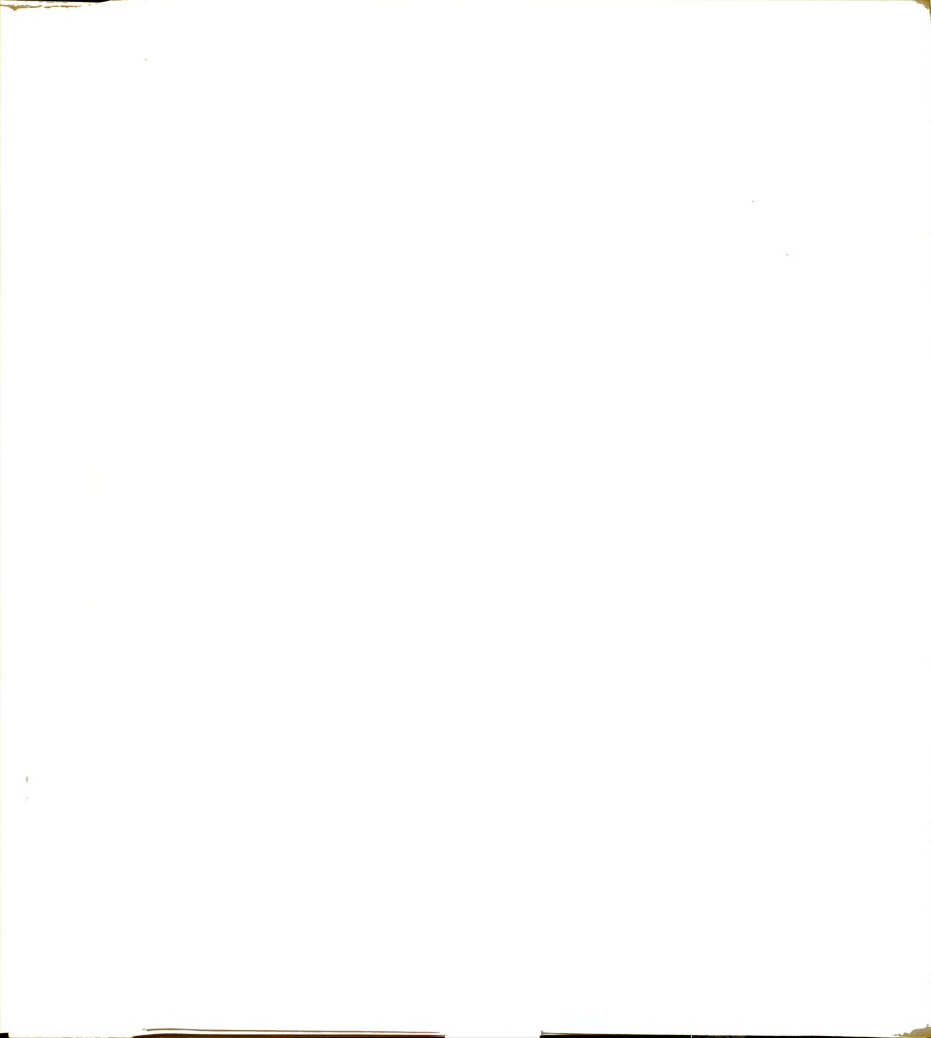
37	RH	27/2	2.00	0.1357	0.1327	0.0030
38	RH	29/2	0.50	0.1413	0.1382	0.0031
39	RH	31/2	0.12	0.1477	0.1430	0.0047
40	RH	33/2	0.02	0.1583	0.1469	0.0114
41	RH	35/2	0.02	0.1604	0.1499	0.0105
42	RH	37/2	0.00	0.1723	0.1519	0.0204
43	P1	1/2	0.00	-0.0000	0.0113	-0.0113
44	P1	3/2	0.00	-0.0000	0.0114	-0.0114
45	P1	5/2	0.00	-0.0000	0.0115	-0.0115
46	P1	7/2	0.00	-0.0000	0.0117	-0.0117
47	P1	9/2	0.00	-0.0000	0.0121	-0.0121
48	P1	11/2	0.00	-0.0000	0.0127	-0.0127
49	P1	13/2	0.00	-0.0000	0.0136	-0.0136
50	P1	15/2	0.00	-0.0000	0.0149	-0.0149
51	P1	17/2	0.00	-0.0000	0.0165	-0.0165
52	P1	19/2	0.00	-0.0000	0.0185	-0.0185
53	P1	21/2	0.00	-0.0000	0.0211	-0.0211
54	P2	1/2	0.00	-0.0000	0.0000	-0.0000
55	P2	3/2	0.00	-0.0000	0.0000	-0.0000
56	P2	5/2	0.00	-0.0000	0.0001	-0.0001
57	P2	7/2	0.00	-0.0000	0.0002	-0.0002
58	P2	9/2	0.00	-0.0000	0.0003	-0.0003
59	P2	11/2	0.00	-0.0000	0.0004	-0.0004
60	P2	13/2	0.00	-0.0000	0.0004	-0.0004
61	P2	15/2	0.00	-0.0000	0.0008	-0.0008
62	P2	17/2	0.00	-0.0000	0.0010	-0.0010
63	P2	19/2	0.00	-0.0000	0.0012	-0.0012
64	P2	21/2	0.00	-0.0000	0.0015	-0.0015
65	R1	1/2	0.00	0.0000	-0.0113	0.0113
66	R1	3/2	0.00	0.0000	-0.0113	0.0113
67	R1	5/2	0.00	0.0000	-0.0112	0.0112
68	R1	7/2	0.00	0.0000	-0.0111	0.0111
69	R1	9/2	0.00	0.0000	-0.0110	0.0110
70	R1	11/2	0.00	0.0000	-0.0108	0.0108
71	R1	13/2	0.00	0.0000	-0.0107	0.0107
72	R1	15/2	0.00	0.0000	-0.0105	0.0105
73	R1	17/2	0.00	0.0000	-0.0103	0.0103
74	R1	19/2	0.00	0.0000	-0.0100	0.0100
75	R1	21/2	0.00	0.0000	-0.0098	0.0098
76	R2	1/2	0.00	0.0000	-0.0000	0.0000
77	R2	3/2	0.00	0.0000	-0.0001	0.0001
78	R2	5/2	0.00	0.0000	-0.0002	0.0002
79	R2	7/2	0.00	0.0000	-0.0003	0.0003
80	R2	9/2	0.00	0.0000	-0.0004	0.0004
81	R2	11/2	0.00	0.0000	-0.0005	0.0005
82	R2	13/2	0.00	0.0000	-0.0007	0.0007
83	R2	15/2	0.00	0.0000	-0.0009	0.0009
84	R2	17/2	0.00	0.0000	-0.0011	0.0011
85	R2	19/2	0.00	0.0000	-0.0014	0.0014
86	R2	21/2	0.00	0.0000	-0.0017	0.0017
87	Q1	1/2	0.00	0.0000	-0.0227	0.0227
88	Q1	3/2	0.00	0.0000	-0.0453	0.0453
89	Q1	5/2	0.00	0.0000	-0.0679	0.0679
90	Q1	7/2	0.00	0.0000	-0.0903	0.0903



91	Q1	9/2	0.00	0.0000	-0.1124	0.1124
92	Q1	11/2	0.00	0.0000	-0.1344	0.1344
93	Q1	13/2	0.00	0.0000	-0.1560	0.1560
94	Q1	15/2	0.00	0.0000	-0.1773	0.1773
95	Q1	17/2	0.00	0.0000	-0.1982	0.1982
96	Q1	19/2	0.00	0.0000	-0.2186	0.2186
97	Q1	21/2	0.00	0.0000	-0.2385	0.2385
98	Q1	23/2	0.00	0.0000	-0.2579	0.2579
99	Q1	25/2	0.00	0.0000	-0.2766	0.2766
100	Q1	27/2	0.00	0.0000	-0.2947	0.2947
101	Q1	29/2	0.00	0.0000	-0.3121	0.3121
102	Q1	31/2	0.00	0.0000	-0.3288	0.3288
103	Q2	3/2	0.00	0.0000	-0.0001	0.0001
104	Q2	5/2	0.00	0.0000	-0.0002	0.0002
105	Q2	7/2	0.00	0.0000	-0.0005	0.0005
106	Q2	9/2	0.00	0.0000	-0.0011	0.0011
107	Q2	11/2	0.00	0.0000	-0.0018	0.0018
108	Q2	13/2	0.00	0.0000	-0.0029	0.0029
109	Q2	15/2	0.00	0.0000	-0.0044	0.0044
110	Q2	17/2	0.00	0.0000	-0.0063	0.0063
111	Q2	19/2	0.00	0.0000	-0.0087	0.0087
112	Q2	21/2	0.00	0.0000	-0.0116	0.0116
113	Q2	23/2	0.00	0.0000	-0.0150	0.0150
114	Q2	25/2	0.00	0.0000	-0.0191	0.0191
115	Q2	27/2	0.00	0.0000	-0.0239	0.0239
116	Q2	29/2	0.00	0.0000	-0.0294	0.0294
117	Q2	31/2	0.00	0.0000	-0.0357	0.0357

S.D. = 0.0028





MICHIGAN STATE UNIVERSITY LIBRARIES



3 1293 03083 1840