# HIGH RESOLUTION ABSORPTION, ZEEMAN, AND MAGNETIC ROTATION SPECTRA OF NITROGEN DIOXIDE IN THE NEAR INFRARED

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MELVIN D. OLMAN

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This is to certify that the

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HIGH RESOLUTION ABSORPTION, ZEEMAN, AND
MAGNETIC ROTATION SPECTRA OF
NITROGEN DIOXIDE IN THE NEAR INFRARED

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Melvin D. Olman

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Major professor

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ABSTRACT

HIGH RESOLUTION ABSORPTION, ZEEMAN,
AND MAGNETIC ROTATION SPECTRA OF
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by Melvin D. Olman

The absorption, Zeeman, and magnetic rotation spectra of the (1,0,1) and (2,0,1) vibration-rotation bands of nitrogen dioxide have been obtained using Michigan State University's high resolution ($\sim$0.03 $cm^{-1}$ at 4200 $cm^{-1}$), near-infrared spectrometer. Improved values of the ground state molecular constants of $^{14}NO_2$ and $^{15}NO_2$ have been obtained from an analysis of combined ground state combination differences and microwave transition frequencies. Accurate upper state rotational and centrifugal distortion constants and band origins have been obtained for the (1,0,1) and (2,0,1) bands of $^{14}NO_2$ and $^{15}NO_2$. In addition, the change in the effective spin-rotation coupling constant between the ground and the (2,0,1) vibrational states has been determined for each isotopic species.

Theoretical expressions have been found which give the frequencies and transition probabilities for the Zeeman components of absorption transitions at all magnetic fields. The spectra predicted by these expressions match very closely the details of the experimental spectra at all magnetic fields available.

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In the magnetic rotation spectra the strongest signals are found to come from Q-branch transitions. In the P branches there are one or more series of weaker signals which arise from transitions for which $K_{-1} = 5$, 6, and 7. The relative strengths of the Q- and P-branch signals and the dependence of the Q-branch signals on the magnetic field strength have been qualitatively explained on the basis of the theoretical Zeeman patterns.

# HIGH RESOLUTION ABSORPTION, ZEEMAN, AND MAGNETIC ROTATION SPECTRA OF NITROGEN DIOXIDE IN THE NEAR INFRARED

By

Melvin Dennis Olman

A THESIS

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To MARY

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# INTRODUCTION

Nitrogen dioxide is one of the few stable, paramagnetic molecules with a single unpaired electron, and thus its spectrum and structure have been of interest to investigators for some time. Microwave and far-infrared transition frequencies have been measured and ground state constants for several isotopic forms have been determined by Bird et al.[1,2] and by Lees, Curl, and Baker.[3] Arakawa and Nielsen[4] and Moore[5] have reported the analysis of the medium resolution vibration-rotation bands in the near-infrared, using the symmetric top approximation. Observation of the near-infrared magnetic rotation spectrum of $NO_2$ was reported by Aubel.[6]

The present work reports the analysis of the high resolution absorption, Zeeman, and magnetic rotation spectra of the (1,0,1) and (2,0,1) vibration-rotation bands of $^{14}NO_2$ and $^{15}NO_2$ in the near-infrared. The rotational structure of the absorption bands is analyzed using existing asymmetric rotor theory and yields improved values for the rotational and centrifugal distortion constants of the ground and upper vibrational states. Effective spin-rotation coupling constants are determined from measurements of the zero-field splittings.

As a result of the single unpaired electron, the ground electronic state of the nitrogen dioxide molecule is a $^2\Sigma$ state.[7] The coupling between the electron spin and the molecular rotation removes the degeneracy of the doublet and leads to a splitting of many of the observed transitions. In the presence of an external magnetic field, the coupling between the magnetic moment of the electron and the field leads to a Zeeman splitting of the energy levels and a corresponding splitting of many of the observed transitions.

Expressions which are valid at all field strengths are derived for the frequencies and transition probabilities of the several Zeeman components of an absorption line. Computer plots of the resulting theoretical Zeeman spectra at several field strengths are found to compare well with experimental spectra.

It is found that the strongest magnetic rotation signals arise from Q-branch transitions for which there is a maximum separation of $\Delta M_N=+1$ and $\Delta M_N=-1$ transitions. Weaker signals in the P and R branches are found to come from spin-doublets.

# CHAPTER I

# THEORY

## A. ASYMMETRIC TOP ENERGIES

### Rigid Rotor

The geometry of the planar triatomic molecule $NO_2$ is shown in Fig. 1. The axes of the principal moment of inertia ellipsoid are designated by a, b, and c, and the corresponding principal moments of inertia are designated $I_a$, $I_b$, and $I_c$, with the axes labelled in the conventional way so that $I_a \leq I_b \leq I_c$. The b-axis is the $C_{2v}$ symmetry axis of the molecule.

The general rigid rotor Hamiltonian is

$$H_0 = \frac{P_a^2}{2I_a} + \frac{P_b^2}{2I_b} + \frac{P_c^2}{2I_c} . \qquad (1)$$

A more convenient form for $H_0$, for which the energies are in wavenumbers ($cm^{-1}$), is

$$H_0 = A\, P_a^2 + B\, P_b^2 + C\, P_c^2 , \qquad (2)$$

where the reciprocal moments of inertia, A, B, and C, are the usual rotational molecular constants and are related to the principal moments by $A = \hbar/(4\pi c I_a)$, etc.

The molecule is classified according to the values of A, B, and C.

A spherical top molecule has A = B = C, and the resulting expression for the energy depends only on the total rotational angular momentum quantum number N.

A symmetric top molecule has two of the three reciprocal moments equal. The axis associated with the third, unique, moment is the symmetric top axis. Here the energy depends upon N and the projection of N along the symmetric top axis K. Since the energy depends only on the square of K, levels having K non-zero are doubly degenerate. Molecules for which A > B = C, "a" being the unique axis, are called prolate symmetric tops, while those having A = B > C are oblate symmetric tops.

In the general case of an asymmetric top molecule each of the reciprocal moments is unique (A > B > C). Since the resulting asymmetric top Hamiltonian cannot be diagonalized exactly, numerical methods must be used to get the molecular energies.

The degree of asymmetry of the molecule is indicated by Ray's asymmetry parameter,[8] $\kappa = \frac{2B-A-C}{A-C}$. If $B \simeq C$ ($\kappa \to -1$), the molecule is called a prolate asymmetric top, while if $B \simeq A$ ($\kappa \to +1$), it is called an oblate asymmetric top.

For nitrogen dioxide $\kappa \simeq -0.994$ so that the molecule is nearly an accidentally symmetric prolate top (B = C). For such a case the energy can be written in the form[9]

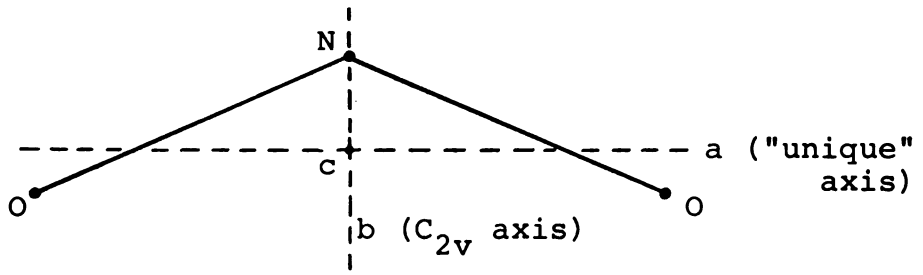
$$W_0 = \frac{B+C}{2} N(N+1) + (A - \frac{B+C}{2})\omega \ , \qquad (3)$$

where $\omega$ is the Wang energy and must be computed numerically.

The manner in which the energies of the lowest rotational levels change as $\kappa$ varies from -1 to +1 is shown in Fig. 2. Although the rotational angular momentum quantum number N is still a good quantum number, the asymmetry lifts the degeneracy in K. The value of K which a given energy level would have in the $\kappa = -1$ (prolate) limit is labelled $K_{-1}$, and its value in the $\kappa = +1$ (oblate) limit is labelled $K_{+1}$. Thus, although K itself is no longer a good quantum number, it is possible to identify a given energy level uniquely by N, $K_{-1}$, and $K_{+1}$, regardless of the degree of the asymmetry. The conventional notation for the identification of a given energy level is $N_{K_{-1}K_{+1}}$. Since nitrogen dioxide is so nearly a prolate symmetric top, K will often be used here to mean $K_{-1}$.

## Centrifugal Distortion Effects

The rigid rotor Hamiltonian contains only terms which depend on the square of the angular momentum components. In an actual molecular system, the rotation of the nuclei leads to a centrifugal stretching of the molecular bonds which requires the inclusion of centrifugal distortion corrections in the Hamiltonian. These correction terms include $P^4$- and $P^6$-type operators.




$\measuredangle$O-N-O = 134°4', $r_s$ = 1.1934 Å

Fig. 1. Geometry of the $NO_2$ molecule. (Structural constants from Bird et al.[1])

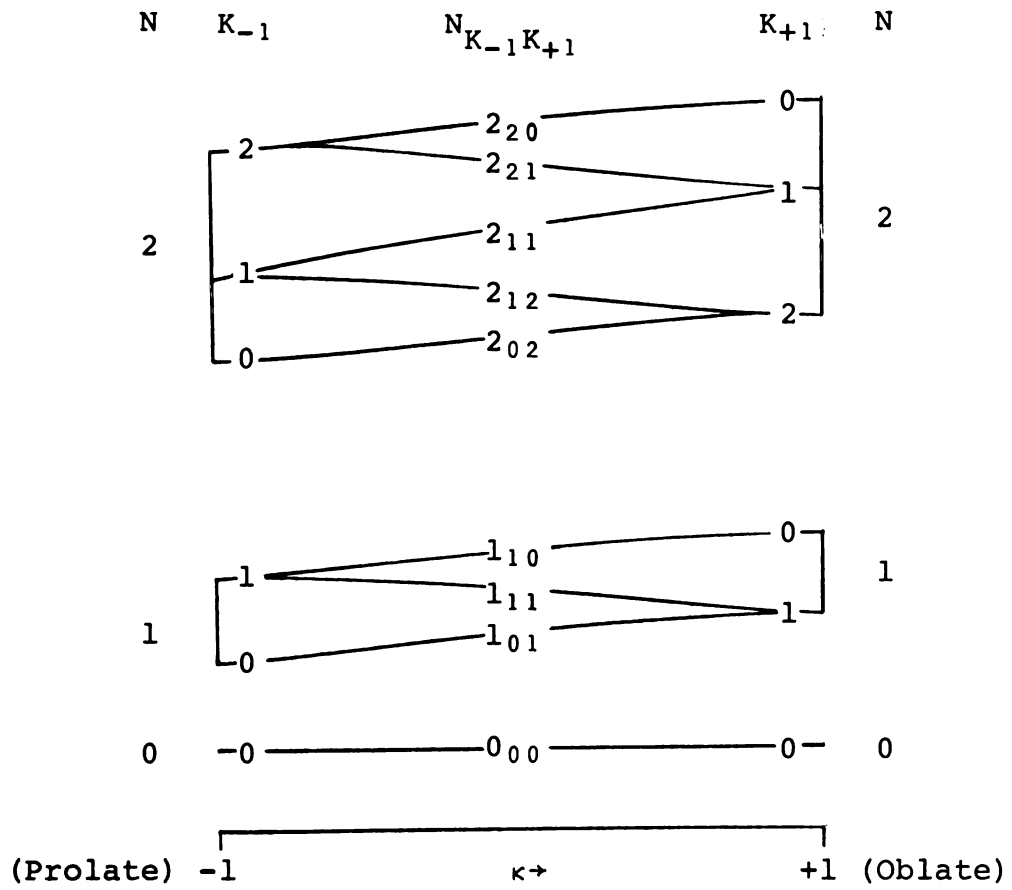



Fig. 2. Asymmetric top energy level diagram.

$P^4$ terms. As summarized by Hill,[10] the general Hamiltonian which takes care of the vibrationally independent $P^4$-type terms is

$$H_1 = \sum \tau_{\mu\nu\xi\zeta} P_\mu P_\nu P_\xi P_\zeta \ . \qquad (4)$$

From the commutation relations for the angular momentum operators and the relationships which develop among the $\tau$'s for a planar molecule,[11] the eighty-one general $\tau$'s are reduced to only four independent $\tau$'s for $NO_2$: $\tau_{aaaa}$, $\tau_{bbbb}$, $\tau_{aabb}$, and $\tau_{abab}$. (When the following expressions are used in the section on the analysis of the data, the $\tau$'s will be referred to as $\tau_1$, $\tau_2$, $\tau_3$, and $\tau_4$, respectively.) Hill[10] has given the resulting energies to first order as

$$W_1 = \tau_{aaaa} X_1 + \tau_{bbbb} X_2 + \tau_{aabb} X_3 + \tau_{abab} X_4 \ , \qquad (5)$$

where

$$X_1 = \frac{1}{16}\Big\{r^2[N^2(N+1)^2 - \delta_1 - 2N(N+1)\delta_2] - (r-2)[2rN(N+1)\langle P_z^2\rangle + 2r\delta_3 - (r-2)\langle P_z^4\rangle]\Big\}$$

$$X_2 = \frac{1}{16}\Big\{(1+s)^2[N^2(N+1)^2 - 2N(N+1)\langle P_z^2\rangle + \langle P_z^4\rangle] - (1-s)^2\delta_1 + 2(1-s^2)[N(N+1)\delta_2 + \delta_3]\Big\}$$

$$X_3 = \frac{1}{8}\Big\{(1+s)[rN^2(N+1)^2 - 2(r-1)N(N+1)\langle P_z^2\rangle + (r-2)\langle P_z^4\rangle] + r[(1-s)\delta_1 - 2sN(N+1)\delta_2] - 2[1+s(1-r)]\delta_3\Big\}$$

$$X_4 = \frac{1}{2}\Big\{N(N+1)\langle P_z^2\rangle - \langle P_z^4\rangle - \delta_3\Big\}$$

and

$$\delta_1 = (2\omega\langle P_z^2\rangle - \langle P_z^4\rangle - \omega^2)/b_p^2$$

$$\delta_2 = (\langle P_z^2\rangle - \omega)/b_p$$

$$\delta_3 = (\omega\langle P_z^2\rangle - \langle P_z^4\rangle)/b_p$$

$$b_p = \frac{C-B}{2A-B-C} = \frac{\kappa-1}{\kappa+3}$$

$$r = C_e^2/A_e^2, \quad s = C_e^2/B_e^2 .$$

$A_e$, $B_e$, and $C_e$ are the equilibrium rotational constants. Since equilibrium values of the constants are not known for $NO_2$, it is necessary to use ground state values in the calculation of r and s.

The commutation relations reduce some of the $P^4$ terms in Eq. (5) to have the $P^2$ dependence of the terms in Eq. (2) so that the observed rotational constants, which we shall label A', B', and C', are related to the reciprocal moments, A, B, and C, by the following equations, which are due to Hill:[10]

$$\begin{aligned} A' &= A - \tfrac{1}{2}\,\tau_{abab} \\ B' &= B - \tfrac{1}{2}\,\tau_{abab} \\ C' &= C + \tfrac{3}{4}\,\tau_{abab} . \end{aligned} \tag{6}$$

Chung and Parker have cited an expression[12] for the theoretical value of $\tau_{abab}$:

$$\tau_{abab} = -\frac{16\,A_eB_eC_e}{\omega_3^2} \tag{7}$$

where $\omega_3$ is the normal frequency of the $\nu_3$ vibrational mode.

Although the $\tau$'s as defined in Eq. (5) are independent of the vibrational state involved, one expects different vibrational states to have different centrifugal distortion energies. At the present time this can only be handled empirically by allowing the $\tau$'s to have different values in different vibrational states.

$P^6$ terms. In the analysis of the observed data, which includes transitions with N as large as 48 and $K_{-1}$ as large as 8, it is found that a good fit of the data requires the inclusion of $P^6$-type terms, in addition to the $\tau$'s. After Pierce, Di Cianni, and Jackson,[13] the following semi-empirical expression is used:

$$W_2 = H_N N^3(N+1)^3 + H_{NK} N^2(N+1)^2 \langle P_z^2 \rangle + H_{KN} N(N+1) \langle P_z^4 \rangle + H_K \langle P_z^6 \rangle , \tag{8}$$

where the H's are to be determined experimentally.

We can now write the rotational energy of a prolate asymmetric rotor molecule as

$$\begin{aligned} W = {} & \frac{B+C}{2} N(N+1) + (A - \frac{B+C}{2}) \omega \\ & + \tau_{aaaa} \chi_1 + \tau_{bbbb} \chi_2 + \tau_{aabb} \chi_3 + \tau_{abab} \chi_4 \\ & + H_N N^3(N+1)^3 + H_{NK} N^2(N+1)^2 \langle P_z^2 \rangle + H_{KN} N(N+1) \langle P_z^4 \rangle + H_K \langle P_z^6 \rangle . \end{aligned} \tag{9}$$

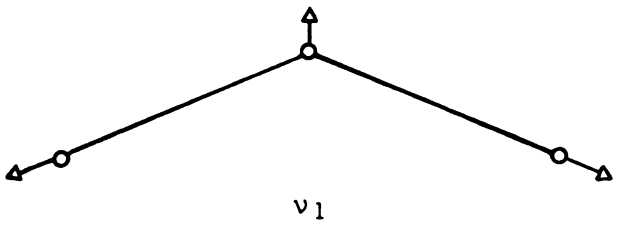
In this expression A, B, and C, the four $\tau$'s, and the four H's are constants only for a given vibrational state.

## Vibration-Rotation Bands

The vibration-rotation bands observed here are due to transitions originating in the ground vibrational state and terminating in a vibrationally excited state. Being a triatomic molecule, nitrogen dioxide has three vibrational degrees of freedom so that there are three normal modes of vibration. These are shown schematically in Fig. 3. A vibrational state is labelled $(n_1,n_2,n_3)$, where $n_i$ denotes the number of quanta of $\nu_i$ which have been excited for a molecule in that state. It is important here to recognize that the third normal mode $\nu_3$ corresponds to an unsymmetrical vibration so that the vibrational wavefunction for a state in which an odd number of $\nu_3$ quanta have been excited must be anti-symmetric, whereas the vibrational wavefunctions for all other states, including the ground state, are symmetric.[14]

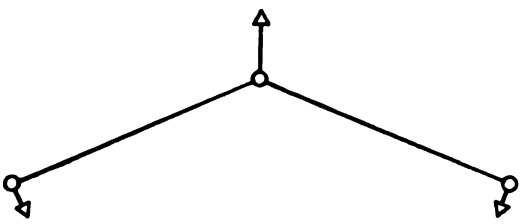
By far the strongest bands observed here, and the only ones analyzed, have an odd number of $\nu_3$ quanta in the upper vibrational states. From Figs. 1 and 3 it can be seen that for these bands the change in the dipole moment must be parallel to the a-axis. Thus they are called type-A or, since the a-axis is the limiting symmetric top axis, parallel bands. The selection rules for such bands are $\Delta N = 0, \pm 1$ and $\Delta K_{-1} = 0$. (With finite asymmetry, $\Delta K_{-1} = \pm 2$ transitions are allowed, but for $\kappa = -0.994$, their intensities are effectively zero.)

Fundamental Frequency
(Arakawa and Nielsen[4])



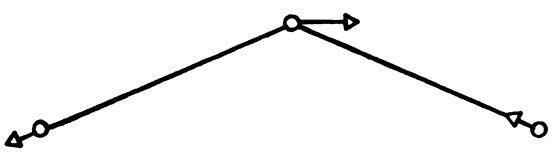
$\nu_1$

1318 $cm^{-1}$



$\nu_2$

749.8 $cm^{-1}$



$\nu_3$

1617.8 $cm^{-1}$

Fig. 3. Normal modes of vibration for $NO_2$.

The $C_{2v}$ symmetry of the molecule, along with the zero nuclear spin of the $^{16}O$ nuclei, requires that only states having a totally symmetric wavefunction be populated.[15] This requires that for the ground state, only rotational levels for which the rotational wavefunction is symmetric ($K_{+1} + K_{-1}$ even) be populated, while the upper vibrational states of the bands observed can only have anti-symmetric ($K_{+1} + K_{-1}$ odd) rotational levels populated. The result is that only half of the energy levels are populated, and thus only half of the allowed transitions occur in each vibration-rotation band.

## Analysis

The frequency $\nu$ of a rotational line in a vibration-rotation band is given by

$$\nu = \nu_0 + W'(N',K'_{-1},K'_{+1}) - W''(N'',K''_{-1},K''_{+1}) \qquad (10)$$

where the primes refer to the upper vibrational state and the double primes to the ground state. $\nu_0$ is the energy difference between the N=0 levels of the excited and ground vibrational states and is called the band origin. For the observed nitrogen dioxide bands the selection rules require that

$$\Delta N = N' - N'' = 0, \pm 1$$

$$\Delta K = \Delta K_{-1} = K'_{-1} - K''_{-1} = 0 \ .$$

Since only half of the allowed transitions occur, no

ambiguity will arise from the use of symmetric top notation to identify the transitions, ${}^{\Delta K}\Delta N_K(N)$, where the letters P, Q, and R denote $\Delta K$ or $\Delta N = -1$, 0, and +1, respectively, and N and K refer to the ground state values of N and $K_{-1}$. The branches within a band are ${}^{Q}P_K(N)$, ${}^{Q}Q_K(N)$, and ${}^{Q}R_K(N)$, or more commonly, the P, Q, and R branches.

By taking differences between appropriate transition frequencies within an absorption band, one can obtain information about rotational energy differences within just the ground or just the upper vibrational state. These are the usual ground or upper state combination differences (GSCD or USCD).

The analysis of a set of combination differences proceeds as follows: Following the procedure used by Hill,[10] the rigid rotor energy expression, Eq. (3), can be rewritten as

$$\begin{aligned} W_0 &= \frac{B+C}{2} N(N+1) + \left(A - \frac{B+C}{2}\right)\omega \\ &= \zeta A + \xi \frac{B+C}{2} + \eta \frac{B-C}{2} \end{aligned} \tag{11}$$

where $\zeta = \dfrac{\partial W_0}{\partial A}$, $\xi = \dfrac{\partial W_0}{\partial \left(\frac{B+C}{2}\right)}$, and $\eta = \dfrac{\partial W_0}{\partial \left(\frac{B-C}{2}\right)}$.

Since the Wang energy can be written as[16]

$$\omega = K_{-1}^2 + \sum_n c_n b_p^n \tag{12}$$

where $b_p = \dfrac{C-B}{2A-B-C}$, and the $c_n$ are numerical coefficients,

the following expressions can be obtained for $\zeta$, $\xi$, and $\eta$:

$$\zeta = \frac{\partial W_0}{\partial A} = \omega + (A - \frac{B+C}{2}) \frac{\partial \omega}{\partial A}$$

$$= \omega + (A - \frac{B-C}{2}) \frac{\partial b_p}{\partial A} \frac{\partial \omega}{\partial b_p}$$

$$= \omega - b_p \frac{\partial \omega}{\partial b_p} \qquad (13\text{-a})$$

$$\xi = \frac{\partial W_0}{\partial (\frac{B+C}{2})} = N(N+1) - \omega + (A - \frac{B+C}{2}) \frac{\partial \omega}{\partial (\frac{B+C}{2})}$$

$$= N(N+1) - \omega + b_p \frac{\partial \omega}{\partial b_p} \qquad (13\text{-b})$$

and $$\eta = \frac{\partial W_0}{\partial (\frac{B-C}{2})} = (A - \frac{B+C}{2}) \frac{\partial W}{\partial (\frac{B-C}{2})} = - \frac{\partial \omega}{\partial b_p} . \qquad (13\text{-c})$$

Using $\frac{\partial W_0}{\partial A} = \langle P_a^2 \rangle = \langle P_z^2 \rangle$ (since the limiting symmetric top axis is the z-axis) leads to

$$\zeta = \langle P_z^2 \rangle$$

$$\xi = N(N+1) - \langle P_z^2 \rangle \qquad (14)$$

$$\eta = (\langle P_z^2 \rangle - \omega)/b_p .$$

A computer subroutine[17] is used to calculate the Wang energies and the values of $\langle P_z^2 \rangle$, $\langle P_z^4 \rangle$, and $\langle P_z^6 \rangle$ for a given set of A, B, and C values. A program was written to use these values and calculate $W_0$, $\zeta$, $\xi$, and $\eta$ for each level of interest.

If one has a set of observed energy levels and trial values of the rotational constants, $\bar{A}$, $\bar{B}$, and $\bar{C}$, a set of calculated energy levels can be formed using Eq. (3) or Eq. (11). From the differences between the observed and calculated energy levels, corrections to the rotational constants can be obtained by a least-squares fit to an equation of the form

$$W(N,K_{-1},K_{+1})_{obs} - W(N,K_{-1},K_{+1})_{calc} = \zeta\cdot\Delta A + \xi\cdot\Delta\left(\frac{B+C}{2}\right) + \eta\cdot\Delta\left(\frac{B-C}{2}\right), \tag{15}$$

where $\Delta A = A - \bar{A}$, etc., and A, B, and C are the new experimental values of the rotational constants as determined by the least squares fit. By using these as new trial values, a refined set of constants can be determined. To include centrifugal distortion terms, Eq. (15) must be modified as follows:

$$W_{obs} - W_{calc} = \zeta\cdot\Delta A + \xi\cdot\Delta\left(\frac{B+C}{2}\right) + \eta\cdot\Delta\left(\frac{B-C}{2}\right) + \sum_i \chi_i \Delta\tau_i + N^3(N+1)^3\Delta H_N + N^2(N+1)^2\langle P_z^2\rangle\Delta H_{NK} + N(N+1)\langle P_z^4\rangle\Delta H_{KN} + \langle P_z^6\rangle\Delta H_K . \tag{16}$$

Here, the $\Delta\tau$'s and $\Delta H$'s are the corrections to the trial values of the $\tau$'s and H's. Since $\zeta$, $\xi$, $\eta$, $\langle P_z^2\rangle$, $\langle P_z^4\rangle$, $\langle P_z^6\rangle$ depend only on the trial values of A, B, and C, it is not necessary to have starting values of the $\tau$'s and H's.

If their trial values are all taken as zero, the least squares fit will give their final values directly.

In practice, only the differences of energy levels in a given vibrational state are observed through the combination differences. Thus Eq. (16) has to be changed to the following:

$$
\begin{aligned}
[W_1 - W_2]_{obs} - [W_1 - W_2]_{calc} = \\
&(\zeta_1-\zeta_2)\Delta A + (\xi_1-\xi_2)\Delta\left(\frac{B+C}{2}\right) + (\eta_1-\eta_2)\Delta\left(\frac{B-C}{2}\right) \\
&+ \sum_i (\chi_{i_1}-\chi_{i_2})\Delta\tau_i + [N_1^3(N_1+1)^3 - N_2^3(N_2+1)^3]\Delta H_N \\
&+ [N_1^2(N_1+1)^2\langle P_z^2\rangle_1 - N_2^2(N_2+1)^2\langle P_z^2\rangle_2]\Delta H_{NK} \\
&+ [N_1(N_1+1)\langle P_z^4\rangle_1 - N_2(N_2+1)\langle P_z^4\rangle_2]\Delta H_{KN} \\
&+ [\langle P_z^6\rangle_1 - \langle P_z^6\rangle_2]\Delta H_K
\end{aligned}
\qquad (17)
$$

where the subscripts 1 and 2 refer to the two states whose energy difference has been measured. It was found that only one or two iterations of A, B, and C were necessary before no further changes were made.

If a fit of observed frequencies is desired, Eq. (17) must be modified to include the band origin $\nu_0$ and to take into account the fact that there are different sets of rotational constants associated with states 1 and 2. If a calculated set of frequencies, $\nu_{calc}$, is formed using Eq. (10), corrections are found for $\nu_0$ and for the upper and

ground state constants by applying the following equation to each observed frequency:

$$
\begin{aligned}
\nu_{obs} - \nu_{calc} = \\
&\Delta\nu_0 + \zeta'\Delta A' + \xi'\Delta\left(\frac{B'+C'}{2}\right) + \eta'\Delta\left(\frac{B'-C'}{2}\right) + \sum_i \chi_i'\Delta\tau_i' \\
&+ N'^3(N'+1)^3\Delta H_N' + N'^2(N'+1)^2\langle P_z^2\rangle'\Delta H_{NK}' \\
&+ N'(N'+1)\langle P_z^4\rangle'\Delta H_{KN}' + \langle P_z^6\rangle'\Delta H_K' \qquad (18) \\
&- \zeta''\Delta A'' - \xi''\Delta\left(\frac{B''+C''}{2}\right) - \eta''\Delta\left(\frac{B''-C''}{2}\right) - \sum_i \chi_i''\Delta\tau_i'' \\
&- N''^3(N''+1)^3\Delta H_N'' - N''^2(N''+1)^2\langle P_z^2\rangle''\Delta H_{NK}'' \\
&- N''(N''+1)\langle P_z^4\rangle''\Delta H_{KN}'' - \langle P_z^6\rangle''\Delta H_K'' \ .
\end{aligned}
$$

Here the primes and double primes refer to quantities in the upper and ground vibrational states, respectively, and the $\Delta$'s again refer to changes in the various coefficients.

Several computer programs were written to aid in the reduction and analysis of the raw frequency data. They are described in more detail in Appendix I. SCAN reduces raw data from the Hydel system[18] to fringe numbers. CALFIT determines the calibration constants for each chart. These are input to SCAN to convert the fringe numbers to frequencies. SPECFIT fits observed frequencies directly to determine the band origin and the rotational constants for the two vibrational levels involved in a given band. CDSORT finds the differences of transitions within a given band

having a common upper (lower) level to form GSCD (USCD). CDFIT fits GSCD or USCD to determine rotational constants for a given vibrational level.

## B. SPIN-ROTATION COUPLING

### Energies

So far, only the contribution that the rotational angular momentum of the nuclei makes to the total angular momentum of the molecule has been considered. In addition, there are the contributions of the spin of the single umpaired electron $\underline{S}$ and the non-zero nuclear spin of the nitrogen atom $\underline{I}$. The contribution of the nuclear spin to the energy levels is too small to be observed with the resolution available in the near infrared and is therefore neglected. With this simplification the total angular momentum is taken as that resulting from the addition of $\underline{N}$ and $\underline{S}$. In the absence of external fields, $\underline{N}$ and $\underline{S}$ couple to form $\underline{J}$, the total angular momentum of the molecule. Since $S = \frac{1}{2}$, the possible values of J are $N + \frac{1}{2}$ and $N - \frac{1}{2}$.

Henderson,[19] Lin,[7] and Raynes[20] have discussed the mechanism of the coupling between $\underline{N}$ and $\underline{S}$ in great detail. Ignoring off-diagonal terms in N as having little effect on the energies, Lin[7] writes the spin-rotation Hamiltonian as

$$H_{SR} = \frac{\underline{N}\cdot\underline{S}}{N(N+1)} \sum_{ij} \varepsilon_{ij} N_i N_j \ , \quad \varepsilon_{ij} = \varepsilon_{ji} \ , \tag{19}$$

where the $\varepsilon$'s are spin-rotation coupling coefficients which must be determined experimentally. Using the symmetric top approximation that the off-diagonal elements of the $\varepsilon$ tensor are zero, and that $\varepsilon_{bb} = \varepsilon_{cc}$, Lin's results can be written as

$$H_{SR} = \left[\frac{\varepsilon_{bb}+\varepsilon_{cc}}{2} + (\varepsilon_{aa} - \frac{\varepsilon_{bb}+\varepsilon_{cc}}{2}) \frac{K^2}{N(N+1)}\right] \underline{N}\cdot\underline{S} \ . \qquad (20)$$

Since the microwave value of $\frac{\varepsilon_{bb}+\varepsilon_{cc}}{2}$ is $\sim$-0.0015 $cm^{-1}$,[3] the first term was dropped as being insignificant. The resulting Hamiltonian is

$$H_{SR} = \mathcal{K}_{SR}\, \underline{N}\cdot\underline{S} \qquad (21)$$

$$\text{where } \mathcal{K}_{SR} = \frac{\varepsilon K^2}{N(N+1)} \quad \text{and} \quad \varepsilon = \varepsilon_{aa} - \frac{\varepsilon_{bb}+\varepsilon_{cc}}{2} \ . \qquad (22)$$

At an early stage in the analysis, the above symmetric top approximation was tested by using the complete expression of Curl and Kinsey[21] for an asymmetric top. It was found that the fit to the experimental results did not change and that values of $\varepsilon_{bb}$ and $\varepsilon_{cc}$ could not be determined as being significantly different from zero.

$$\text{Since} \quad \langle J|\underline{N}\cdot\underline{S}|J\rangle = \tfrac{1}{2}\,[J(J+1) - N(N+1) - S(S+1)], \qquad (23)$$

the spin-rotation energies can be written as

$$\begin{aligned} W^{+}_{SR} &= \mathcal{K}_{SR}\, \frac{N}{2} \\ W^{-}_{SR} &= -\,\mathcal{K}_{SR}\, \frac{(N+1)}{2} \end{aligned} \qquad (24)$$

where $W_{SR}^{\pm}$ is the energy which must be added to Eq. (9) to get the energy of the $J^{\pm}=N\pm\frac{1}{2}$ state. The coupling of $\underline{N}$ and $\underline{S}$ to form $\underline{J}$ and the splitting of a typical level are shown at the left side of Fig. 4 (page 28). Note that the splitting given by Eq. (24) is not symmetrical about the zero-spin positions.

## Analysis

For electric dipole transitions the selection rule for J is $\Delta J = 0, \pm 1$, but transitions having $\Delta J = \Delta N$ are by far the strongest. Transitions having $\Delta J \neq \Delta N$ have not been observed in the infrared spectra of $NO_2$ so that all observed transitions are either $W^+ \rightarrow W^+$ or $W^- \rightarrow W^-$. Thus the spin-rotation splittings of the observed spectral lines arise only from differences in the splittings of the levels which are involved in the transitions. If $\Delta J \neq \Delta N$ transitions can be found, they will provide direct observation of the spin splittings in the upper and lower states.

If $\nu$ represents the frequency of a given transition in the absence of spin-rotation splitting, the frequencies of the observed spin-split components ($\Delta J = \Delta N$) will be given by

$$\nu^{\pm} = \nu + W_{SR}^{\pm}(\varepsilon',N',K') - W_{SR}^{\pm}(\varepsilon'',N'',K'') \quad . \tag{25}$$

From this

$$\begin{aligned} \nu^{+} - \nu^{-} = {} & W_{SR}^{+}(\varepsilon',N',K') - W_{SR}^{+}(\varepsilon'',N'',K'') \\ & - W_{SR}^{-}(\varepsilon',N',K') + W_{SR}^{-}(\varepsilon'',N'',K'') \quad . \end{aligned} \tag{26}$$

Substitution of Eq. (24) gives

$$\nu^+ - \nu^- = \frac{K^2(N'+\frac{1}{2})}{N'(N'+1)}\,\varepsilon' - \frac{K^2(N''+\frac{1}{2})}{N''(N''+1)}\,\varepsilon'' \,, \qquad (27)$$

where the fact that $\Delta K = 0$ has been used.

If the assumption is made that isotopic substitution does not change the electronic structure,[20] the following expressions can be used:

$$\frac{\varepsilon^*_{aa}}{\varepsilon_{aa}} = \frac{A^*}{A} \,, \quad \frac{\varepsilon^*_{bb}}{\varepsilon_{bb}} = \frac{B^*}{B} \,, \quad \frac{\varepsilon^*_{cc}}{\varepsilon_{cc}} = \frac{C^*}{C} \,, \qquad (28)$$

where the starred and unstarred coefficients correspond to the values of the coefficient for two isotopes of a given molecule. Thus, $\frac{^{14}\varepsilon_{aa}}{^{15}\varepsilon_{aa}} = \frac{^{14}A}{^{15}A}$, etc., for each vibrational level.

Since the effective $\varepsilon$ observed is nearly equal to $\varepsilon_{aa}$, the approximation

$$\frac{\varepsilon^*}{\varepsilon} = \frac{A^*}{A} \qquad (29)$$

should be valid.

A program SPINFIT (see Appendix I) was written to take input values of $(\nu^+ - \nu^-)$, K, N, $\Delta$N, and a weight for each observed splitting and perform a least squares fit to get values for $\varepsilon''$ and $\varepsilon'$. Data for $^{14}NO_2$ and $^{15}NO_2$ can be fit separately to get the $\varepsilon$'s for each molecule, or Eq. (29) can be used to combine the two sets of data for the determination of $\frac{^{14}\varepsilon}{^{14}A} = \frac{^{15}\varepsilon}{^{15}A}$ for each vibrational state.

Due to the asymmetry of the splitting of the energy levels, the spin-free frequency of a line is not midway between the two components, i.e., $\nu \neq \frac{\nu^+ + \nu^-}{2}$. Thus it is necessary to use the results of an analysis of the data with Eq. (27) to correct the components of the doublet to a single spin-free frequency. Only after this has been done can the transition be included with the data which is fit to Eq. (17) or (18) to determine rotational and other constants.

## C. ZEEMAN EFFECT

### Energies

In the absence of external forces and torques, molecular energy levels are independent of the molecule's orientation in space so that there is a degeneracy of (2J+1) associated with each energy level. This corresponds to the (2J+1) possible values of $M_J$, the component of the total angular momentum J on the space-fixed Z-axis.

The nitrogen dioxide molecule has a magnetic moment $\underline{\mu}$ which arises predominantly from the magnetic moment of the unpaired spin, $\underline{\mu} = -\frac{g_s \mu_B}{\hbar} \underline{S}$. Here, $g_s$ is the free electron g-factor, and $\mu_B$ is the Bohr magneton. Aside from its function in the spin-rotation coupling, the small magnetic moment arising from the end-over-end rotation of the molecule can be ignored.

In the presence of an external magnetic field there will be a torque on the magnetic moment of the molecule

which will lift the $M_J$ degeneracy through the action of the Zeeman Hamiltonian

$$H_Z = - \underline{\mu} \cdot \underline{H} = \frac{g_s \mu_B}{\hbar} \underline{S} \cdot \underline{H} = 2 \Delta\nu \, S_Z \, , \qquad (30)$$

where $\Delta\nu = \frac{1}{2} g_s \mu_B H$ is in $cm^{-1}$ and H is in gauss ($\frac{1}{2} g_s \mu_B = 4.6754 \times 10^{-5}$ $cm^{-1}$/gauss).

At low field strengths the $\underline{N} \cdot \underline{S}$ coupling predominates so that J is still a valid quantum number, and the wavefunction for rotation and spin may be written

$$|N,S,J^{\pm},M_J\rangle \, . \qquad (31)$$

These are eigenvectors of the spin-rotation Hamiltonian [Eq. (21)], but not of the Zeeman Hamiltonian [Eq. (30)].

At higher field strengths the $\underline{S} \cdot \underline{H}$ coupling predominates, and J is no longer a meaningful quantum number. $\underline{N}$ and $\underline{S}$ couple to the field (Z-axis) separately so that the wavefunction may be written

$$|N,M_N,S,M_S\rangle \, . \qquad (32)$$

These are eigenvectors of the Zeeman Hamiltonian but not of the spin-rotation Hamiltonian.

For the general case of any magnetic field strength, an expression is found for the spin-rotation and Zeeman energies. The approach is similar to that originally developed by E. L. Hill for diatomic molecules and first published by Almy in his treatment of the $^2\Sigma$ state of OH.[22]

The perturbation Hamiltonian is taken as

$$H_{SR,Z} = H_{SR} + H_Z \ . \tag{33}$$

Since $H_{SR}$ is diagonal only in the $|J,M_J\rangle$ representation, and $H_Z$ is diagonal only in the $|M_N,M_S\rangle$ representation, $H_{SR,Z}$ will have both diagonal and off-diagonal matrix elements in either of these representations. Thus the perturbation energies will have to be found by diagonalization of the energy matrix in either of these two representations.

$|J,M_J\rangle$ representation. Initially the $|J^{\pm},M_J\rangle$ representation was used. Using vector coupling coefficients for the addition of two angular momenta, the two $|J^{\pm},M_J\rangle$ wavefunctions can be expressed as linear combinations of the two $|M_N,M_S=\pm\frac{1}{2}\rangle$ wavefunctions:[23]

$$\begin{aligned} |J^+,M_J\rangle &= \left[\frac{N+M_J+\frac{1}{2}}{2N+1}\right]^{\frac{1}{2}} |M_N,M_S=\tfrac{1}{2}\rangle + \left[\frac{N-M_J+\frac{1}{2}}{2N+1}\right]^{\frac{1}{2}} |M_N',M_S=-\tfrac{1}{2}\rangle \\ |J^-,M_J\rangle &= -\left[\frac{N-M_J+\frac{1}{2}}{2N+1}\right]^{\frac{1}{2}} |M_N,M_S=\tfrac{1}{2}\rangle + \left[\frac{N+M_J+\frac{1}{2}}{2N+1}\right]^{\frac{1}{2}} |M_N',M_S=-\tfrac{1}{2}\rangle \end{aligned} \tag{34}$$

where the values of $M_N$ and $M_N'$ are fixed at $M_N = M_J-\frac{1}{2}$ and $M_N' = M_J+\frac{1}{2}$ . Using the $|J^{\pm},M_J\rangle$ wavefunctions as the basis wavefunctions leads to a two-by-two matrix in which the off-diagonal elements couple only levels having the same value of $M_J = M_N + M_S$:

$$
\begin{array}{c|cc}
 & |J^+,M_J\rangle & |J^-,M_J\rangle \\
\hline
\langle J^+,M_J| & K_{SR}\frac{N}{2} + \Delta\nu\left(\frac{M_J}{N+\frac{1}{2}}\right) & -\Delta\nu\left[1-\left(\frac{M_J}{N+\frac{1}{2}}\right)^2\right]^{\frac{1}{2}} \\
\langle J^-,M_J| & -\Delta\nu\left[1-\left(\frac{M_J}{N+\frac{1}{2}}\right)^2\right]^{\frac{1}{2}} & -K_{SR}\frac{N+1}{2} - \Delta\nu\left(\frac{M_J}{N+\frac{1}{2}}\right)
\end{array}
\tag{35}
$$

Since the $|J^-,M_J\rangle$ level does not exist for $M_J = \pm J^+$, the $|J^+,M_J\rangle$ level with $M_J = \pm J^+$ must be treated separately. The resulting energy expressions for $M_J \neq \pm J^+$ are

$$
W_{SR,Z}(N,J^{\pm},M_J) = -\frac{K_{SR}}{4} \pm \frac{1}{2}\left[(\Delta W)^2 + 4(\Delta\nu)(\Delta W)\frac{M_J}{(N+\frac{1}{2})} + 4(\Delta\nu)^2\right]^{\frac{1}{2}} , \tag{36-a}
$$

while for $M_J = \pm J^+$

$$
W_{SR,Z}(N,J^+,M_J=\pm J^+) = \frac{K_{SR}}{2}N \pm \Delta\nu . \tag{36-b}
$$

Here, $\Delta W$ is the zero-field separation of the $J^+$ and $J^-$ levels, and

$$
\Delta W = W^+_{SR} - W^-_{SR} = K_{SR}(N+\tfrac{1}{2}) .
$$

$|M_N,M_S\rangle$ representation. In the consideration of selection rules and transition probabilities for the Zeeman components of a transition, it was found necessary to use the $|M_N,M_S\rangle$ representation. Using the inverse of Eq. (34)[24]

$$|M_N, M_S=+\tfrac{1}{2}> = \left[\frac{N+M_N+1}{2N+1}\right]^{\frac{1}{2}} |J^+, M_J=M_N+\tfrac{1}{2}> - \left[\frac{N-M_N}{2N+1}\right]^{\frac{1}{2}} |J^-, M_J=M_N+\tfrac{1}{2}>$$

$$|M_N+1, M_S=-\tfrac{1}{2}> = \left[\frac{N-M_N}{2N+1}\right]^{\frac{1}{2}} |J^+, M_J=M_N+\tfrac{1}{2}> + \left[\frac{N+M_N+1}{2N+1}\right]^{\frac{1}{2}} |J^-, M_J=M_N+\tfrac{1}{2}> , \tag{37}$$

the following energy matrix is obtained:

$$\begin{array}{c|cc} & |M_N,+\tfrac{1}{2}> & |M_N+1,-\tfrac{1}{2}> \\ \hline <M_N,+\tfrac{1}{2}| & \frac{K_{SR}}{2} M_N + \Delta\nu & \frac{K_{SR}}{2}[N^2+N-M_N^2-M_N]^{\frac{1}{2}} \\ <M_N+1,-\tfrac{1}{2}| & \frac{K_{SR}}{2}[N^2+N-M_N^2-M_N]^{\frac{1}{2}} & -\frac{K_{SR}}{2}(M_N+1) - \Delta\nu \end{array} . \tag{38}$$

Again, only levels having the same value of $M_J = M_N + M_S$ are coupled. The resulting energies are

$$W_{SR,Z}(N,M_N,\pm\tfrac{1}{2}) = -\frac{K_{SR}}{4} \pm \left[(\Delta\nu)^2 + K_{SR}(\Delta\nu)(M_N\pm\tfrac{1}{2}) + \tfrac{1}{4}(\Delta W)^2\right]^{\frac{1}{2}} \tag{39-a}$$

except that

$$W_{SR,Z}(N,M_N=\pm N,\pm\tfrac{1}{2}) = \frac{K_{SR}}{2} N \pm \Delta\nu . \tag{39-b}$$

As should be the case, these equations are equivalent to Eqs. (36), and if all that is desired is a knowledge of the level structure at various field strengths, either representation may be used.

Figure 4 gives the identification of the several energy sub-levels having a given N at low magnetic field strengths

(Zeeman coupling) and at high magnetic field strengths (Paschen-Back coupling). The requirements that $M_J = M_N + M_S$ remain constant for each sub-level and that energy sub-levels having the same $M_J$ value may not cross as the field is changed are sufficient to connect the sub-levels from the low- to the high-field limits in a unique way. The dotted lines connect the high- and low-field positions of each level.

Figure 5 shows the predicted Zeeman splittings as a function of field strengths for the sub-levels of the $3_{31}$ level of the ground state of $^{14}NO_2$.

## Intensities and Frequencies

Before the preceeding energy expressions can be used to predict the appearance of the Zeeman spectrum of a band at various fields, it is necessary to find the intensities of the various Zeeman components within a given rotational transition. For these, it is necessary to find the transition probability.

The transition probability for an electric dipole transition from a state $|n\rangle$ to a state $|m\rangle$ is given by

$$|\langle n|\vec{M}|m\rangle|^2 \equiv |\langle n|M_X|m\rangle|^2 + |\langle n|M_Y|m\rangle|^2 + |\langle n|M_Z|m\rangle|^2, \quad (40)$$

where $\vec{M}$ is the electric dipole moment of the system and $M_X$, $M_Y$, and $M_Z$ are the components of $\vec{M}$ in the space-fixed coordinate system. These components can be expressed in terms of the components in the body-fixed coordinate system, $M_x$,

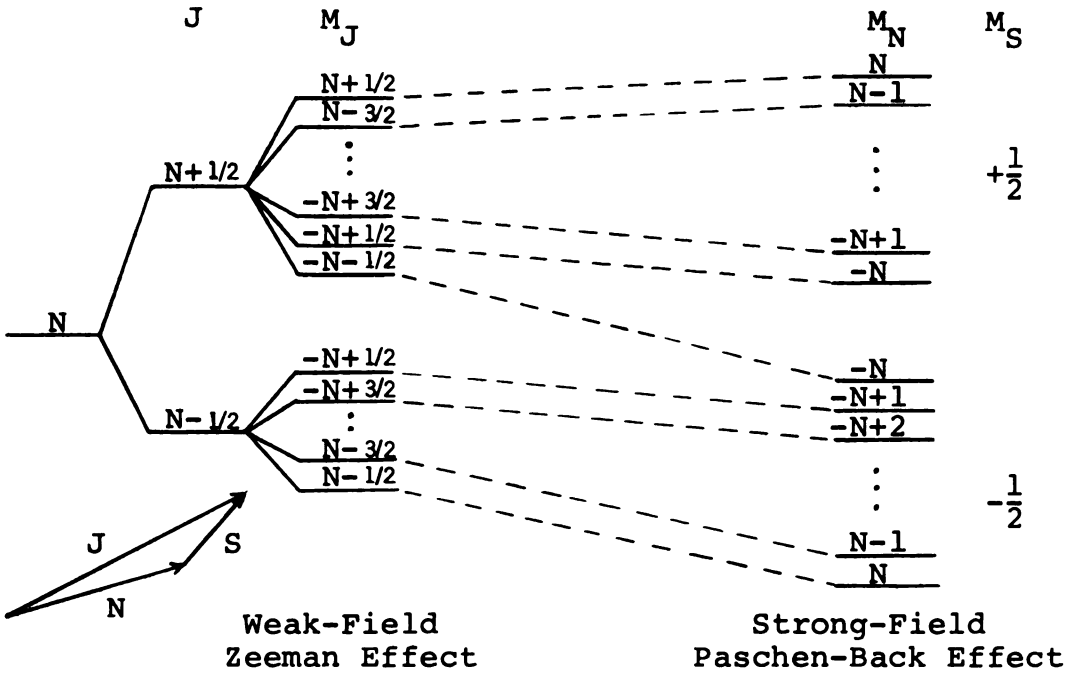



Fig. 4. Energy level splittings and identifications at weak and strong magnetic fields.

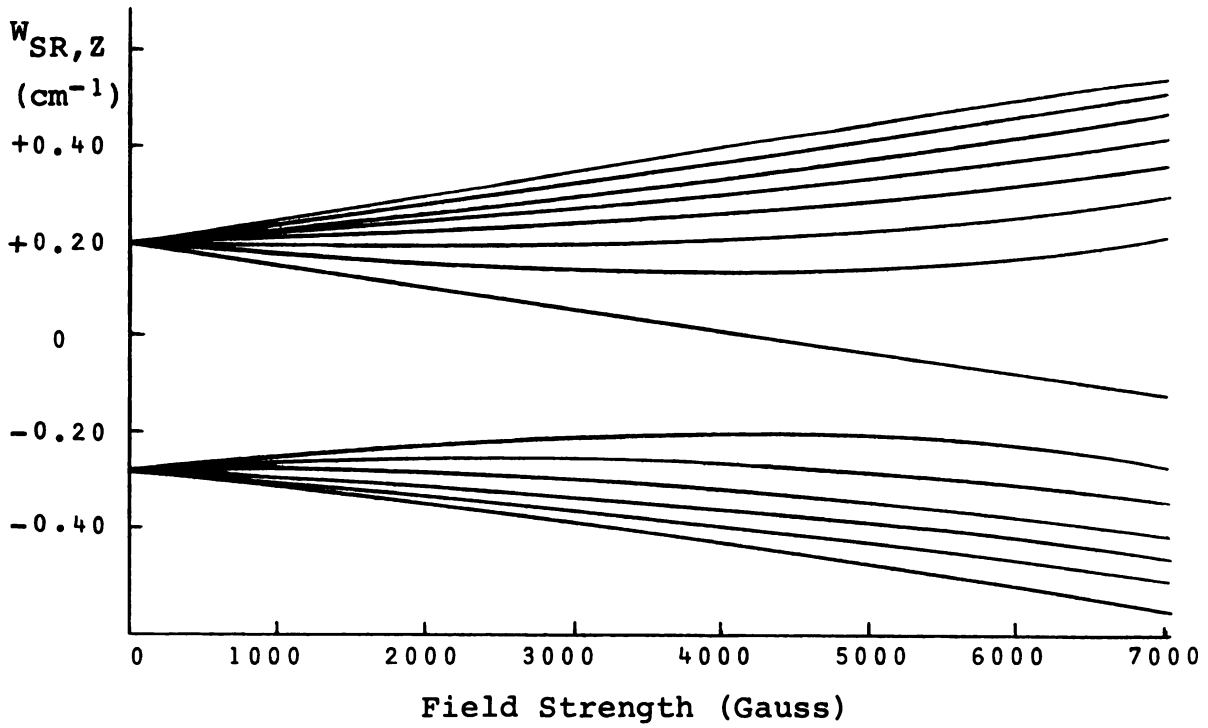



Fig. 5. Predicted splitting for the $3_{31}$ level of the ground state of $^{14}NO_2$.

$M_y$, and $M_z$, through the direction cosines as given by Cross, Hainer, and King:[25]

$$\langle n|M_A|m\rangle = \sum_\alpha M_\alpha (\Phi_{A\alpha})_{n,m} \ . \tag{41}$$

Here, A = X, Y, or Z and α = x, y, or z.

Since the only $NO_2$ bands observed with reasonable intensity are type-A bands, where the change in the dipole moment is along the a- or z-axis, it will be assumed that the dipole moment has a non-zero component along only the z-axis, i.e., $M_x = M_y = 0$, $M_z \neq 0$.

Although Cross, Hainer, and King and others write the matrix elements of $\vec{M}$ as $\langle J,K,M_J|\vec{M}|J',K',M_J'\rangle$, they are treating the special case of zero-spin angular momentum so that by J they mean the total <u>rotational</u> angular momentum N. Thus, the matrix elements, $\langle N,K,M_N|\vec{M}|N',K',M_N'\rangle$, must be formed in order to calculate the transition probabilities.

With this understanding, the $(\Phi_{A\alpha})_{n,m}$ can be written

$$(\Phi_{A\alpha})_{N,K,M_N;N',K',M_N'} = (\Phi_{A\alpha})_{N;N'}(\Phi_{A\alpha})_{N,K;N',K'}(\Phi_{A\alpha})_{N,M_N;N',M_N'} \ , \tag{42}$$

where the $\Phi_{A\alpha}$ on the right hand side have been given by Cross, Hainer, and King.[25]

Since all of the Zeeman work reported here is done with a longitudinal magnetic field, only transitions having $\Delta M_N = M_N' - M_N = \pm 1$ will occur. With this restriction, all

matrix elements of $M_Z$ vanish. Combining this with the fact that $\Delta K = 0$ for the transitions of interest and using Eq. (42) reduces Eq. (41) to

$$\langle N,K,M_N|M_A|N',K,M_N\pm1\rangle = M_z(\Phi_{Az})_{N;N'}(\Phi_{Az})_{N,K;N',K}(\Phi_{Az})_{N,M_N;N',M_N\pm1} \cdot \tag{43}$$

The $\Phi_{Az}$ of interest are given in Table I.

The resulting matrix elements of $M_X$ and $M_Y$ for the R, Q, and P branches are

$$\begin{aligned}
&\langle N,M_N|M_X|N+1,M_N\pm1\rangle = \pm i\langle N,M_N|M_Y|N+1,M_N\pm1\rangle \\
&\quad = \pm M_z\left\{[(N+1)^2-K^2](N\pm M_N+1)(N\pm M_N+2)\right\}^{\frac{1}{2}}[4(N+1)^2(2N+1)(2N+3)]^{-\frac{1}{2}} \\
&\langle N,M_N|M_X|N,M_N\pm1\rangle = \pm i\langle N,M_N|M_Y|N,M_N\pm1\rangle \\
&\quad = M_zK[(N\mp M_N)(N\pm M_N+1)]^{\frac{1}{2}}[4N^2(N+1)^2]^{-\frac{1}{2}} \\
&\langle N,M_N|M_X|N-1,M_N\pm1\rangle = \pm i\langle N,M_N|M_Y|N-1,M_N\pm1\rangle \\
&\quad = \mp M_z[(N^2-K^2)(N\mp M_N)(N\mp M_N-1)]^{\frac{1}{2}}[4N^2(4N^2-1)]^{-\frac{1}{2}} ,
\end{aligned} \tag{44}$$

where the quantum number K has been left out of the wavefunctions since it is a constant for any given transition ($\Delta K = 0$).

Wavefunctions. In order to calculate the intensities of Zeeman components at all magnetic field strengths, it is necessary to find an expression for the mixing of the $|N,K,M_N\rangle$ wavefunctions which arises from $H_{SR,Z}$. (The mixing

Table I. Direction cosine matrix elements for prolate symmetric top.[a]

| | N' | | |
|---|---|---|---|
| | N+1 | N | N-1 |
| $(\Phi_{Az})_{N;N'}$ | $\{4(N+1)[(2N+1)(2N+3)]^{\frac{1}{2}}\}^{-1}$ | $[4N(N+1)]^{-1}$ | $[4N(4N^2-1)^{\frac{1}{2}}]^{-1}$ |
| $(\Phi_{Az})_{N,K;N',K}$ | $2[(N+K+1)(N-K+1)]^{\frac{1}{2}}$ | $2K$ | $-2[N^2-K^2]^{\frac{1}{2}}$ |
| $(\Phi_{Xz})_{N,M_N;N',M_N\pm1}$ $= \pm i(\Phi_{Yz})$ | $\pm[(N\pm M_N+1)(N\pm M_N+2)]^{\frac{1}{2}}$ | $[(N\mp M_N)(N\pm M_N+1)]^{\frac{1}{2}}$ | $\pm[(N\mp M_N)(N\mp M_N-1)]^{\frac{1}{2}}$ |

[a]From Reference 25.

of these wavefunctions which is caused by the asymmetry of the molecule will be ignored here since $NO_2$ is so nearly a symmetric top.) Since $\langle M_S|\vec{M}|M_S'\rangle$ is zero unless $M_S' = M_S$, the wavefunctions of Eq. (32) are the wavefunctions which should be used to calculate the transition probabilities.

In the absence of a magnetic field the correct mixing of these wavefunctions to represent a given energy level is just that given by Eq. (34). As the magnetic field is applied, the mixing will decrease until at high fields a given energy level will be described by either $|N,M_N,S,+\frac{1}{2}\rangle$ or $|N,M_N,S,-\frac{1}{2}\rangle$, in which case the intensities will be given by the usual symmetric top equations.[26]

An alternate approach is to treat the spin-rotation coupling as a perturbation. In the absence of the perturbation, the wavefunctions are $|N,M_N,S,\pm\frac{1}{2}\rangle$. The perturbation acts to mix the wavefunctions to produce the wavefunctions $|J^{\pm},M_J\rangle$. The amount of the mixing is determined by the ratio of the perturbation energy to the Zeeman energy. Thus the mixing is a maximum at zero magnetic field and decreases as the field is increased. In the limit of high fields the perturbation energy is much less than the Zeeman energy, and there is effectively no mixing.

If the degeneracy of two states, $|1\rangle$ and $|2\rangle$, is lifted by the action of a perturbation V, with matrix elements

$$\begin{array}{c|cc} & |1\rangle & |2\rangle \\ \hline \langle 1| & V_{11} & V_{12} \\ \langle 2| & V_{21} & V_{22} \end{array} , \qquad (45)$$

the resulting perturbation energies are

$$E_i = \frac{V_{11}+V_{22}}{2} \pm \left[\frac{1}{4}(V_{11}-V_{22}) + V_{12}V_{21}\right]^{\frac{1}{2}} , \qquad (46)$$

where the upper sign gives $E_1$ and the lower sign gives $E_2$. Application of this to the matrices given in Eq. (35) or (38) gives Eq. (36-a) or (39-a).

The perturbation will also cause a mixing of the wavefunctions for the two states. This can be written as

$$\begin{aligned} |1) &= C_{11}|1\rangle + C_{12}|2\rangle \\ |2) &= C_{21}|1\rangle + C_{22}|2\rangle , \end{aligned} \qquad (47)$$

where $|n)$ denotes the resulting wavefunction for the level which had the wavefunction $|n\rangle$ in the absence of the perturbation. The $C_{ij}$ are determined[27] by

$$\begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix} \begin{pmatrix} C_{1i} \\ C_{2i} \end{pmatrix} = E_i \begin{pmatrix} C_{1i} \\ C_{2i} \end{pmatrix} \qquad (48)$$

and the normalization condition,

$$C_{1i}^2 + C_{2i}^2 = 1 . \qquad (49)$$

From this results

$$\begin{aligned} C_{11} &= \pm\left[1 + \left(\frac{V_{21}}{V_{22}-E_1}\right)^2\right]^{-\frac{1}{2}}, \\ C_{21} &= -\left(\frac{V_{21}}{V_{22}-E_1}\right) C_{11} , \end{aligned} \qquad (50)$$

$$C_{22} = \pm \left[ 1 + \left( \frac{V_{12}}{V_{11}-E_2} \right)^2 \right]^{-\frac{1}{2}}, \text{ and}$$

$$C_{12} = - \left( \frac{V_{12}}{V_{11}-E_2} \right) C_{22} .$$

The choice of $\pm$ must be consistent with the phase convention used in the evaluation of the $V_{ij}$. It will be shown later that the upper sign must be used.

Transition probabilities. Comparison of the matrices in Eqs. (38) and (45) shows that for the calculation of the transition probabilities for the Zeeman components, the $V_{ij}$ are

$$\begin{aligned} V_{11} &= \frac{K_{SR}}{2} M_N + \Delta\nu \\ V_{22} &= - \frac{K_{SR}}{2} (M_N+1) - \Delta\nu \\ V_{12} &= V_{21} = \frac{K_{SR}}{2} [N^2+N-M_N{}^2-M_N]^{\frac{1}{2}}, \end{aligned} \tag{51}$$

and the $E_i$ are

$$\begin{aligned} E_1 &= W_{SR,Z}(N,M_N,+\tfrac{1}{2}) \\ E_2 &= W_{SR,Z}(N,M_N+1,-\tfrac{1}{2}) . \end{aligned} \tag{52}$$

From these expressions, the $C_{ij}$ can be calculated using Eq. (50). Eq. (47) becomes

$$|N,M_N,+\tfrac{1}{2}) = C_{11}|N,M_N,+\tfrac{1}{2}> + C_{12}|N,M_N+1,-\tfrac{1}{2}> \tag{53-a}$$

$$|N,M_N+1,-\tfrac{1}{2}) = C_{21}|N,M_N,+\tfrac{1}{2}> + C_{22}|N,M_N+1,-\tfrac{1}{2}> . \tag{53-b}$$

For convenience, Eq. (53-b) is rewritten

$$|N,M_N,-\tfrac{1}{2}) = C^*_{21}|N,M_N-1,+\tfrac{1}{2}> + C^*_{22}|N,M_N,-\tfrac{1}{2}> \ , \qquad (53\text{-}c)$$

where $C^*_{21}$ and $C^*_{22}$ are equal to $C_{21}$ and $C_{22}$ with $M_N$ replaced by $(M_N-1)$ throughout. This replacement must be made in the $V_{ij}$ and $E_i$ also, yielding $V^*_{ij}$ and $E^*_i$.

$$C^*_{11} = \pm\left[1+\left(\frac{V^*_{21}}{V^*_{22}-E^*_1}\right)^2\right]^{-\frac{1}{2}}, \quad C^*_{21} = -\left(\frac{V^*_{21}}{V^*_{22}-E^*_1}\right)C^*_{11}$$

$$C^*_{22} = \pm\left[1+\left(\frac{V^*_{12}}{V^*_{11}-E^*_2}\right)^2\right]^{-\frac{1}{2}}, \quad C^*_{12} = -\left(\frac{V^*_{12}}{V^*_{11}-E^*_2}\right)C^*_{22}$$

$$V^*_{11} = \frac{\kappa_{SR}}{2}(M_N-1) + \Delta\nu \qquad (54)$$

$$V^*_{12} = \frac{\kappa_{SR}}{2}\left[N^2+N-M_N{}^2+M_N\right]^{\frac{1}{2}}$$

$$E^*_2 = W_{SR,Z}(N,M_N,-\tfrac{1}{2})$$

From Fig. 5 it can be seen that at zero field

$$|N,M_N,\pm\tfrac{1}{2}) = |J^{\pm},M_J=M_N\pm\tfrac{1}{2}> \ , \qquad (55\text{-}a)$$

except that

$$|N,M_N=-N,-\tfrac{1}{2}) = |J^+,M_J=-J^+> \ . \qquad (55\text{-}b)$$

By calculating the $C_{ij}$ at zero field, substituting the results in Eqs. (53-a,c), and comparing with Eq. (34) using Eq. (55), the phases for the $C_{ij}$ in Eq. (50) can be fixed:

$C_{11}$ and $C_{22}$ are $\geq 0$ .

Writing the resulting ground state wavefunctions as

$$|N'',M_N'',+\tfrac{1}{2}) = C_{11}''|N'',M_N'',+\tfrac{1}{2}> + C_{12}''|N'',M_N''+1,-\tfrac{1}{2}> \qquad (56\text{-a})$$

$$|N'',M_N'',-\tfrac{1}{2}) = C_{21}^{*''}|N'',M_N''-1,+\tfrac{1}{2}> + C_{22}^{*''}|N'',M_N'',-\tfrac{1}{2}> \qquad (56\text{-b})$$

and those for the upper state as

$$|N',M_N',+\tfrac{1}{2}) = C_{11}'|N',M_N',+\tfrac{1}{2}> + C_{12}'|N',M_N'+1,-\tfrac{1}{2}> \qquad (56\text{-c})$$

$$|N',M_N',-\tfrac{1}{2}) = C_{21}^{*'}|N',M_N'-1,+\tfrac{1}{2}> + C_{22}^{*'}|N',M_N',-\tfrac{1}{2}> \qquad (56\text{-d})$$

leads to the following matrix elements:

$$(N'',M_N'',+\tfrac{1}{2}|\vec{M}|N',M_N',+\tfrac{1}{2}) = C_{11}''C_{11}'<N'',M_N'',+\tfrac{1}{2}|\vec{M}|N',M_N',+\tfrac{1}{2}> + C_{12}''C_{12}'<N'',M_N''+1,-\tfrac{1}{2}|\vec{M}|N',M_N'+1,-\tfrac{1}{2}> \qquad (57\text{-a})$$

$$(N'',M_N'',-\tfrac{1}{2}|\vec{M}|N',M_N',-\tfrac{1}{2}) = C_{21}^{*''}C_{21}^{*'}<N'',M_N''-1,+\tfrac{1}{2}|\vec{M}|N',M_N'-1,+\tfrac{1}{2}> + C_{22}^{*''}C_{22}^{*'}<N'',M_N'',-\tfrac{1}{2}|\vec{M}|N',M_N',-\tfrac{1}{2}> \qquad (57\text{-b})$$

$$(N'',M_N'',+\tfrac{1}{2}|\vec{M}|N',M_N',-\tfrac{1}{2}) = C_{11}''C_{21}^{*'}<N'',M_N'',+\tfrac{1}{2}|\vec{M}|N',M_N'-1,+\tfrac{1}{2}> + C_{12}''C_{22}^{*'}<N'',M_N''+1,-\tfrac{1}{2}|\vec{M}|N',M_N',-\tfrac{1}{2}> \qquad (57\text{-c})$$

$$(N'',M_N'',-\tfrac{1}{2}|\vec{M}|N',M_N',+\tfrac{1}{2}) = C_{21}^{*''}C_{11}'<N'',M_N''-1,+\tfrac{1}{2}|\vec{M}|N',M_N',+\tfrac{1}{2}> + C_{22}^{*''}C_{12}'<N'',M_N'',-\tfrac{1}{2}|\vec{M}|N',M_N'+1,-\tfrac{1}{2}> \; . \qquad (57\text{-d})$$

Consider a general element

$$(n|\vec{M}|m) = c_1\langle 1|\vec{M}|1\rangle + c_2\langle 2|\vec{M}|2\rangle \ . \tag{58}$$

Since

$$\vec{M} = \vec{i}\, M_X + \vec{j}\, M_Y \ ,$$

with $M_Z = 0$ for $\Delta M_N = \pm 1$ transitions, the transition probability for a transition $n \to m$ is

$$\begin{aligned} |(n|\vec{M}|m)|^2 &\equiv |(n|M_X|m)|^2 + |(n|M_Y|m)|^2 \\ &= |c_1\langle 1|M_X|1\rangle + c_2\langle 2|M_X|2\rangle|^2 \\ &\quad + |c_1\langle 1|M_Y|1\rangle + c_2\langle 2|M_Y|2\rangle|^2 \ . \end{aligned} \tag{59}$$

From Eqs. (44) $\langle n|M_Y|m\rangle = \mp i\langle n|M_X|m\rangle$, and $\langle n|M_X|m\rangle$ is real, so that

$$\begin{aligned} |(n|\vec{M}|m)|^2 &= 2[c_1\langle 1|M_X|1\rangle + c_2\langle 2|M_X|2\rangle]^2 \\ &= 2[(n|M_X|m)]^2 \ . \end{aligned} \tag{60}$$

Applying this to Eqs. (57), the transition probabilities for the Zeeman components of transitions in vibration-rotation bands of $NO_2$ are finally

$$\begin{aligned} &|(N'', M_N'', +\tfrac{1}{2}|\vec{M}|N', M_N', +\tfrac{1}{2})|^2 = \\ &\quad 2[C_{11}''C_{11}'\langle N'', M_N'', +\tfrac{1}{2}|M_X|N', M_N', +\tfrac{1}{2}\rangle \\ &\quad + C_{12}''C_{12}'\langle N'', M_N''+1, -\tfrac{1}{2}|M_X|N', M_N'+1, -\tfrac{1}{2}\rangle]^2 \end{aligned} \tag{61-a}$$

$$|(N'',M_N'',-\tfrac{1}{2}|\vec{M}|N',M_N',-\tfrac{1}{2})|^2 =$$

$$2[C_{21}^{*''}C_{21}^{*'}\langle N'',M_N''-1,+\tfrac{1}{2}|M_X|N',M_N'-1,+\tfrac{1}{2}\rangle \qquad (61\text{-b})$$

$$+ C_{22}^{*''}C_{22}^{*'}\langle N'',M_N'',-\tfrac{1}{2}|M_X|N',M_N',-\tfrac{1}{2}\rangle]^2$$

$$|(N'',M_N'',+\tfrac{1}{2}|\vec{M}|N',M_N',-\tfrac{1}{2})|^2 =$$

$$2[C_{11}''C_{21}^{*'}\langle N'',M_N'',+\tfrac{1}{2}|M_X|N',M_N'-1,+\tfrac{1}{2}\rangle \qquad (61\text{-c})$$

$$+ C_{12}''C_{22}^{*'}\langle N'',M_N''+1,-\tfrac{1}{2}|M_X|N',M_N',-\tfrac{1}{2}\rangle]^2$$

$$|(N'',M_N'',-\tfrac{1}{2}|\vec{M}|N',M_N',+\tfrac{1}{2})|^2 =$$

$$2[C_{21}^{*''}C_{11}'\langle N'',M_N''-1,+\tfrac{1}{2}|M_X|N',M_N',+\tfrac{1}{2}\rangle \qquad (61\text{-d})$$

$$+ C_{22}^{*''}C_{12}'\langle N'',M_N'',-\tfrac{1}{2}|M_X|N',M_N'+1,-\tfrac{1}{2}\rangle]^2 \ .$$

The non-zero matrix elements of $M_X$ are given by Eq. (44). From these and Fig. 4 it can be seen that the selection rules on $M_N$ for the perturbed energy states are $\Delta M_N = \pm 1$ for the transitions of Eqs. (61-a) and (61-b), $\Delta M_N = 0, +2$ for those of Eq. (61-c), and $\Delta M_N = 0, -2$ for those of Eq. (61-d).

Frequencies. Application of Eqs. (61) to calculate transition probabilities for P, Q, and R branches ($\Delta N = -1$, 0, and +1) gives non-zero intensities for only those components having $\Delta J = 0, \pm 1$, with $\Delta J = \Delta N$ transitions being much more intense.

For R- and P-branch transitions ($\Delta N = \pm 1$) only one of the weak satellite ($\Delta J \neq \Delta N$) lines occurs at zero field

since the second one would require $\Delta J = \pm 2$, which is not allowed. Correspondingly, Eqs. (61) predict zero transition probabilities for these transitions. In the Q branch ($\Delta N=0$) there are two satellite lines predicted at zero field. As the magnetic field is applied, all of the satellite transitions lose intensity rapidly.

The frequencies for the transitions given in Eqs. (61) are

$$\nu(N'',M_N'',M_S''\rightarrow N',M_N'',M_S') = \nu(\text{asym. rotor}) + W_{SR,Z}(N',M_N',M_S') - W_{SR,Z}(N'',M_N'',M_S''). \quad (62)$$

Analysis. The program ZEMANINT was written to calculate the frequencies using Eq. (62), along with the transition probabilities from Eqs. (61), for the Zeeman components of any specified transition at various magnetic fields.

Figures 6 and 7 show the predicted transition probabilities for a P- and a Q-branch transition, respectively, as calculated by ZEMANINT for fields of 0, 2000, 4000, and 6800 gauss.

## D. MAGNETIC ROTATION SPECTRA

The magnetic rotation spectrum of a gas is the spectrum of radiation which is passed when a sample of the gas has been placed in a longitudinal magnetic field between crossed polarizers. Normally there would be no radiation transmitted through the crossed polarizers, but if the gas exhibits

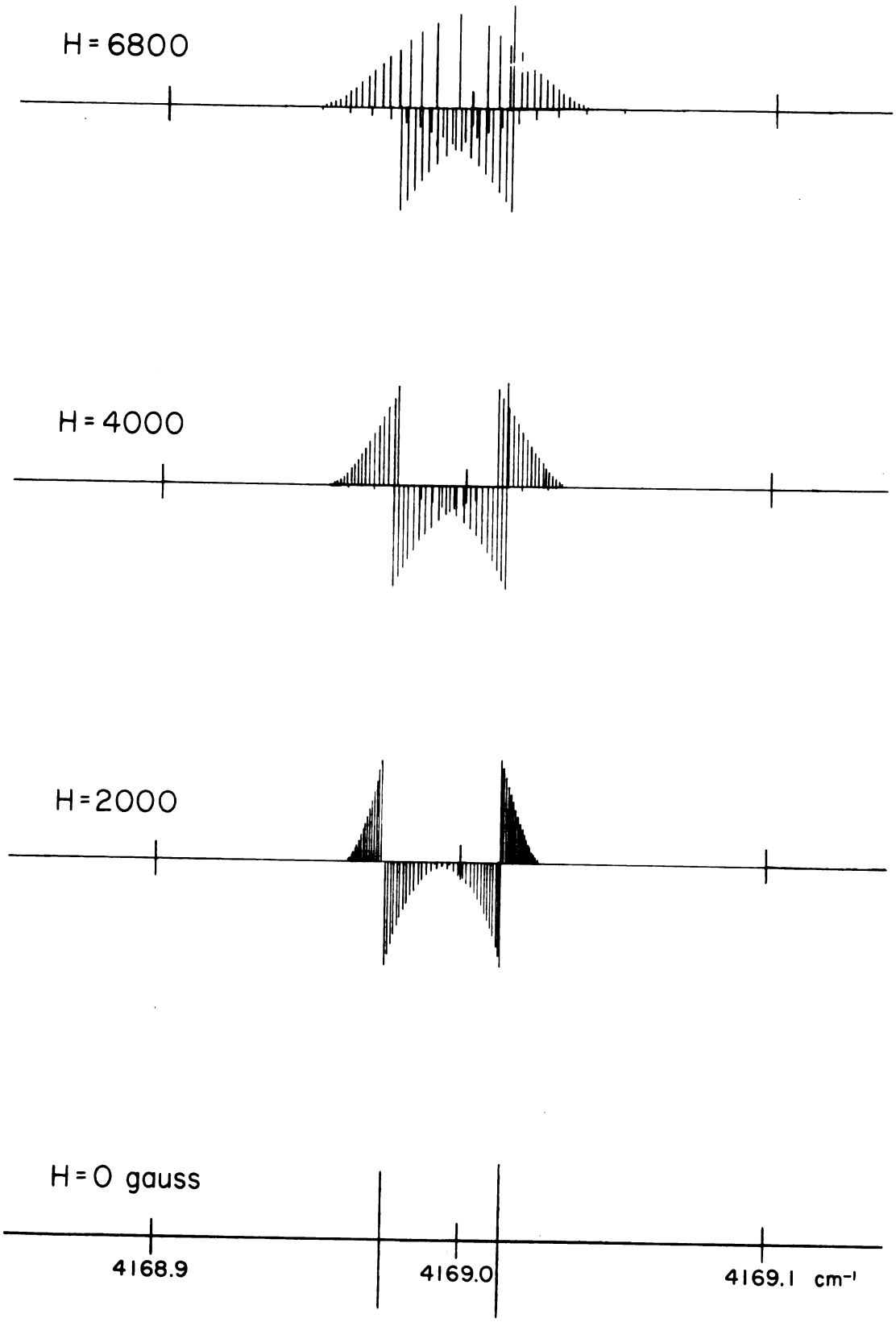



Fig. 6. Predicted Zeeman splittings for the $P_5(10)$ line of the (2,0,1) band of $^{14}NO_2$. The length of each line is proportional to the rotational transition probability for that component. The lengths of the lines for the zero field case have been reduced by a factor of 10 relative to the others. Lines drawn upward (downward) correspond to $\Delta M = +1$ (-1) transitions.

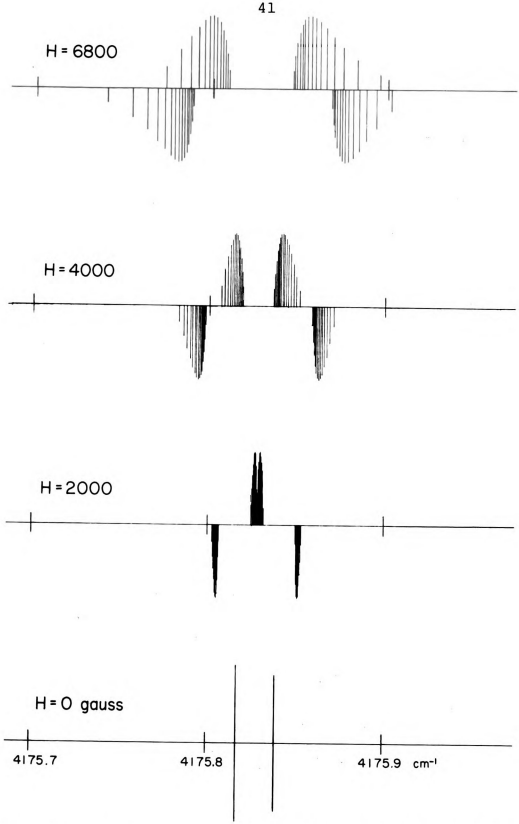



Fig. 7. Predicted Zeeman splittings for the $Q_7(7)$ line of the (2,0,1) band of $^{14}NO_2$. Otherwise this figure is the same as Fig. 6.

magnetic optical activity at certain frequencies, there will be radiation transmitted at those frequencies.

The magnetic rotation signal has been shown to be due to a combination of the Faraday effect and circular dichroism.[28,29,6] An extensive review of "Magnetic Optical Activity" has been presented by Buckingham and Stephens.[30]

In the Faraday effect the plane of polarization of incident radiation is rotated through an angle which is proportional to the difference between the indices of refraction for right and left circularly polarized radiation. Circular dichroism arises from a difference between the absorption coefficients for right and left circular polarization, so that an incident plane-polarized beam becomes somewhat elliptically polarized. Using a semi-classical approach, Aubel[6] shows that Faraday rotation contributes to the magnetic rotation signal only in the wings of absorption lines, where there is very little absorption, while circular dichroism contributes only in regions where there is a significant difference in the amounts of right and left circularly polarized light which is transmitted.

In the region of a nitrogen dioxide absorption line both Faraday rotation and magnetic circular dichroism contribute to the magnetic optical activity, and thus to the magnetic rotation spectrum. Since the $\Delta M_N=+1$ and $\Delta M_N=-1$ transitions are associated with different directions of circular polarization, the magnetic rotation signals depend

on the relative positions and intensities of the Zeeman components of the lines. Thus, it will be useful to refer to Figs. 6 and 7 when the observed magnetic rotation spectra are considered in Chapter II.

# CHAPTER II

# EXPERIMENT AND ANALYSIS

## A. EXPERIMENTAL EQUIPMENT

### Spectrometer

All of the spectra were obtained using the high resolution ($\sim$0.03 $cm^{-1}$ at 4200 $cm^{-1}$), vacuum, grating spectrometer at Michigan State University. Major modifications were made in the optical elements and grating drive-train during an eight month period from September, 1964 to May, 1965. The absorption, magnetic rotation, and initial Zeeman records were obtained during the periods May 25, 1965 to June 24, 1965 and September 23, 1965 to November 2, 1965. At this time the spectrometer was essentially as described by Keck et al.[31] except that the vacuum polarizer assembly and new sources were not yet installed. In December of 1966 after these latter modifications had been completed, additional Zeeman records were obtained when it was found that data at several additional intermediate fields were necessary for a confirmation of the theory.

### Data Reduction

The absorption spectra, recorded on strip charts, were

photographed; then the raw data were digitized using the Hydel system[18] and reduced to absorption frequencies by the computer programs SCAN and CALFIT, which are described in Appendix I.

### Solenoid

A Magnion solenoid capable of fields up to 6800 gauss was used for the Zeeman and magnetic rotation spectra. This solenoid has a seven-inch diameter air core which is forty-eight inches long. Over the central two-thirds of this length, which includes the region of the multiple-traverse absorption cell, the field is uniform to within better than ±2%.

## B. ABSORPTION SPECTRA

### Experimental Conditions

At least two calibrated, high-resolution absorption records were obtained for each of the four bands which have been analyzed and are reported here. The experimental conditions for these records are given in Table II. Each record was measured on the Hydel by two operators so that the absorption frequencies used in the analyses were obtained by averaging at least four different measurements.

### Initial Analysis

The analysis of a given vibration-rotation absorption band started with an initial identification of several low N

Table II. Experimental conditions for absorption spectra.

| Molecule: | $^{14}NO_2$ | | $^{15}NO_2$ | | |
|---|---|---|---|---|---|
| Band: | (1,0,1) | (2,0,1) | (1,0,1) | (2,0,1) | |
| Chart number | 10/21/65<br>10/23/65 | 5/25/65-1,2,3 | 10/28/65<br>10/29/65 | 10/14/65<br>10/15/65 | |
| Pressure (torr) | ∿1 | 15-30 | ∿1 | 10-20 | |
| Path length (m) | 3.15 | 6.30 | 3.15 | 6.30 | |
| Slit width (μ) | 16 | 12 | 16 | 12 | |
| Effective slit width ($cm^{-1}$) | 0.035 | 0.024 | 0.035 | 0.024 | |
| Grating (300 l/mm) | | | | | |
| Angle (degrees) | 30.8-31.8 | 45.6-47.0 | 31.3-32.4 | 46.4-48.0 | |
| Order (for $NO_2$) | 1 | 2 | 1 | 2 | |
| Calibration | | | | | |
| Gas | HCl | CO | HCl | $N_2O$ | CO |
| Band | (1-0) | (2-0) | (1-0) | (3,0,1) | (2-0) |
| Grating order | 1 | 2 | 1 | 3 | 2 |

transitions for which K = 0, 3, 4, ..., since these transitions involve levels which are least affected by the asymmetry and could thus be easily identified by comparison with the structure of a symmetric top parallel band. Holding the ground state rotational constants fixed at the values determined by the microwave analysis,[1,3] it was possible to use SPECFIT (see Appendix I) to determine approximate values for the band origin and upper state rotational constants. From these, a spectrum was predicted, and additional identifications were made. Iteration of this procedure eventually led to a complete analysis of the band, with identification of nearly all of the observed transitions.

For each vibrational state there is a very high correlation between the quantum dependences of $\tau_{aabb}$ and $\tau_{abab}$ which prevents the simultaneous determination of good estimates for these two constants. Equation (7) has been used to fix $\tau_{abab}$ at its theoretical estimate in each case so that a significant estimate of the value of $\tau_{aabb}$ can be found. Since the equilibrium values of the rotational constants are not known, the values for the ground vibrational state are used. (The value of $\omega_3$ is taken from the work of Arakawa and Nielsen.[4])

Included in the final data are the corrected, spin-free frequencies for those transitions which show a resolved spin doubling.

## Ground State Constants

A program CDSORT (see Appendix I) was written to sort through the transitions within each band and form ground state combination differences (GSCD) and upper state combination differences (USCD). Since both bands of each molecule which are analyzed here have the same ground state, the program also forms weighted averages of all of the GSCD found for each molecule. To these are added the reported microwave measurements of ground state energy differences,[1,3] with appropriately high weights.

The infrared data has GSCD for N as high as 48 and K as high as 7, whereas the microwave analysis involves only levels with N up to 22 and K up to 2. Thus it is necessary to use the microwave constants only as very good initial estimates of the ground state constants from which final values are found. In addition, two of the empirical $P^6$ terms, $H_{KN}$ and $H_K$, are found to have significant values for the ground state of $^{14}NO_2$.

Table III summarizes the constants determined by the program CDFIT for the ground states of $^{14}NO_2$ and $^{15}NO_2$ and lists the microwave constants for comparison where available. In each case, Eq. (17) was fit to the combined infrared and microwave data. At first, the rotational constants were held at the microwave values,[1,3] and the $\tau$'s and H's were varied, but the data could not be fit without allowing the rotational constants to vary also.

For $^{14}NO_2$ the rotational constants found here are within the uncertainty quoted by Lees et al.[3] but have significantly smaller uncertainties. This is especially true since the uncertainties determined here are 95% simultaneous confidence intervals which are a factor of 4.0 larger than the standard errors of the coefficients, whereas the uncertainties given for the microwave values are simply the standard errors of the coefficients.

For $^{15}NO_2$ the rotational constants do not agree as well with the microwave values and have somewhat larger uncertainties. The 95% simultaneous confidence intervals are a factor of 3.6 larger than the standard errors of the coefficients.

The observed GSCD used in these fits are listed in Appendix II along with their weights and their deviations from the GSCD calculated using the constants given in Table III.

## Upper State Constants

Rotational and centrifugal distortion constants for the upper state of a vibration-rotation band can be determined in either of two ways--by fitting frequencies or by fitting upper state combination differences (USCD). Once the ground state constants are known, they can be used to subtract the ground state energies from the observed frequencies, leaving just the vibrational and upper state rotational energies, from which the band origin and upper state rotational

Table III. Ground state rotational constants for $NO_2$ (in $cm^{-1}$).

| | $^{14}NO_2$ | |
|---|---|---|
| | Microwave[a] | This Work |
| A | 8.00213 ± 0.00037 | $8.00250_9$ ± 0.00010[b] |
| B | 0.433686 ± 0.000033 | $0.433664_6$ ± 0.000004 |
| C | 0.41044 ± 0.00010 | $0.410492_6$ ± 0.000014 |
| $\tau_{aaaa}$ | $(-9.99 \pm 0.13)\times10^{-3}$ | $(-11.36_5 \pm 0.28)\times10^{-3}$ |
| $\tau_{bbbb}$ | $(-1.382 \pm 0.005)\times10^{-6}$ | $(-1.418_0 \pm 0.023)\times10^{-6}$ |
| $\tau_{aabb}$ | $(6.147 \pm 0.007)\times10^{-5}$ | $(6.90_6 \pm 0.24)\times10^{-5}$ |
| $\tau_{abab}$ | $(-8.182 \pm 0.33)\times10^{-6}$ | $-8.215 \times 10^{-6}$ |
| $H_{KN}$ | | $(-1.1_1 \pm 0.6)\times10^{-7}$ |
| $H_K$ | | $(2.8_4 \pm 1.1)\times10^{-5}$ |
| No. of GSCD | | 162 |
| Std. dev. (I.R. data) | | 0.0048 |

Table III (Continued)

| | $^{15}NO_2$ | |
|---|---|---|
| | Microwave[c] | This Work |
| A | 7.63047 ± 0.00012 | $7.63061_7$ ± 0.00029[b] |
| B | 0.433735 ± 0.000006 | $0.433717_4$ ± 0.000016 |
| C | 0.409440 ± 0.000006 | $0.409491_6$ ± 0.000030 |
| $\tau_{aaaa}$ | $(-9.12 \pm 0.13)\times10^{-3}$ | $(-9.1_5 \pm 0.5)\times10^{-3}$ |
| $\tau_{bbbb}$ | $(-1.382 \pm 0.005)\times10^{-6}$ | $(-1.40_0 \pm 0.04)\times10^{-6}$ |
| $\tau_{aabb}$ | $(5.87 \pm 0.06)\times10^{-5}$ | $(5.8_7 \pm 0.4)\times10^{-5}$ |
| $\tau_{abab}$ | $(-8.16 \pm 0.03)\times10^{-6}$ | $-8.175 \times 10^{-6}$ |
| $H_{KN}$ | | 0.0 |
| $H_K$ | | 0.0 |
| No. of GSCD | | 149 |
| Std. dev. (I.R. data) | | 0.0043 |

[a]Lees, Curl, and Baker.

[b]95% simultaneous confidence intervals.

[c]Bird et al.

constants can be determined using SPECFIT. The alternate method is to use CDSORT to form USCD to which Eq. (17) can be fit to determine the upper state constants.

For the bands analyzed here, the first method is best for several reasons:

(1) For a parallel band ($\Delta K_{-1} = 0$) several of the constants (e.g., A and $H_K$) of a vibrational level cannot be determined by fitting just energy differences. Thus a frequency fit would have to be used to determine these constants and the band origin regardless of how the other constants are determined. There is also the danger that certain of the other constants might not be linearly independent.

(2) The uncertainties of the constants are significantly smaller for this method.

(3) Since it was found (see below) that some of the observed lines do not fit well, possibly indicating the existence of a perturbation, it is more meaningful to fit the energies directly rather than just the energy differences.

The K=3 series of the (2,0,1) band of each molecule could not be fit as well as the rest of the data. For $10 \leqslant N \leqslant 48$ there is a progressive deviation of the observed positions from those predicted by the best constants that can be determined. This deviation is as large as 0.12 $cm^{-1}$ at N = 48. The other series of the (2,0,1) bands and all of

the series of the (1,0,1) bands fit much better with the largest systematic deviations being no larger than 0.07 $cm^{-1}$.

Since GSCD obtained from the K=3 series of the (2,0,1) bands agree with those of the (1,0,1) bands and fit well with the other GSCD, there must be a perturbation of some sort affecting the (2,0,1) vibrational levels. A Coriolis perturbation can probably be ruled out since the nearest-lying band which could have a Coriolis interaction with the (2,0,1) band is $\sim$240 $cm^{-1}$ away. In addition, one would expect a Coriolis interaction to affect more than one of the K levels for a given N. A failure in the analysis scheme, which is based on only a first-order treatment of centrifugal distortion, can be ruled out since the GSCD fit well for all values of N and K used.

Since the deviations of the K=3 series of the (2,0,1) bands are not understood, these series are not included in the final fit to determine the (2,0,1) upper state rotational constants and band origins, although they are used to form the averaged GSCD.

The resulting upper state constants and band origins for the (1,0,1) and (2,0,1) bands of $^{14}NO_2$ and $^{15}NO_2$ are given in Table IV.

## Evaluation of Rotational Constants and Prediction of (0,0,3) and (1,0,3) Rotational Constants

The relations for the vibrational dependence of the rotational constants of a triatomic molecule are written as

Table IV. Upper state rotational constants and band origins for $NO_2$ ($cm^{-1}$).

| | $^{14}NO_2$ | |
|---|---|---|
| | (1,0,1) | (2,0,1) |
| $\nu_0$ | $2906.073_7 \pm 0.006$[a] | $4179.938_3 \pm 0.007$ |
| A | $7.8540_4 \pm 0.0010$ | $7.9264_9 \pm 0.0010$ |
| B | $0.428597_9 \pm 0.000017$ | $0.426283_8 \pm 0.000018$ |
| C | $0.405007_0 \pm 0.000015$ | $0.402253_1 \pm 0.000016$ |
| $\tau_{aaaa}$ | $(-1.155_8 \pm 0.016)\times10^{-2}$ | $(-1.184_9 \pm 0.019)\times10^{-2}$ |
| $\tau_{bbbb}$ | $(-1.430_9 \pm 0.030)\times10^{-6}$ | $(-1.444_3 \pm 0.031)\times10^{-6}$ |
| $\tau_{aabb}$ | $(7.46_9 \pm 0.17)\times10^{-5}$ | $(6.52_1 \pm 0.08)\times10^{-5}$ |
| $\tau_{abab}$ | $-8.215 \times 10^{-5}$ | $-8.215 \times 10^{-5}$ |
| $H_{KN}$ | $(-1.12_9 \pm 0.19)\times10^{-7}$ | 0.0 |
| $H_K$ | $(2.89_3 \pm 0.04)\times10^{-5}$ | $(2.76_8 \pm 0.05)\times10^{-5}$ |
| No. lines identified | 710 | 563 |
| No. lines weighted≠0 | 369 | 286 |
| Std. dev. of fit | 0.0096 | 0.0104 |

Table IV (Continued)

| | $^{15}NO_2$ | |
|---|---|---|
| | (1,0,1) | (2,0,1) |
| $\nu_0$ | $2858.707_1 \pm 0.008$ | $4120.367_3 \pm 0.004$ |
| A | $7.4918_1 \pm 0.0032$ | $7.5398_1 \pm 0.0005$ |
| B | $0.428754_2 \pm 0.000024$ | $0.426487_5 \pm 0.000013$ |
| C | $0.404166_4 \pm 0.000020$ | $0.401450_0 \pm 0.000011$ |
| $\tau_{aaaa}$ | $(-1.41_1 \pm 0.13)\times10^{-2}$ | $(-0.953_3 \pm 0.004)\times10^{-2}$ |
| $\tau_{bbbb}$ | $(-1.363_2 \pm 0.042)\times10^{-6}$ | $(-1.406_8 \pm 0.022)\times10^{-6}$ |
| $\tau_{aabb}$ | $(6.57_2 \pm 0.30)\times10^{-5}$ | $(5.83_7 \pm 0.12)\times10^{-5}$ |
| $\tau_{abab}$ | $-8.175 \times 10^{-5}$ | $-8.175 \times 10^{-5}$ |
| $H_{KN}$ | 0.0 | $(0.82_7 \pm 0.14)\times10^{-7}$ |
| $H_K$ | $(3.6_9 \pm 0.9)\times10^{-5}$ | 0.0 |
| No. lines identified | 482 | 671 |
| No. lines weighted≠0 | 288 | 323 |
| Std. dev. of fit | 0.0118 | 0.0076 |

[a]95% simultaneous confidence intervals throughout.

$$R_{n_1 n_2 n_3} = R_e - \sum_{i=1} \alpha_i^R \left(n_i + \tfrac{1}{2}\right)$$

$$= R_{000} - \sum_{i=1}^{3} \alpha_i^R n_i \ , \tag{63}$$

where R = A, B, or C, and the subscript e denotes the equilibrium value of the constant. From this, the following expressions for $\alpha_1^R$ and $\alpha_3^R$ in terms of the known values of $R_{000}$ , $R_{101}$ , and $R_{201}$ can be obtained:

$$\alpha_1^R = R_{101} - R_{201}$$

$$\alpha_3^R = R_{000} + R_{201} - 2R_{101} \ . \tag{64}$$

The resulting values of these α's for the two molecules are given in Table V. The values of $\alpha_2^R$ cannot be determined since $n_2 = 0$ for all of the bands studied here; thus, equilibrium values of the rotational constants could not be determined.

Frequencies were obtained for the (1,0,3) and (0,0,3) bands of each molecule. The analysis of the (0,0,3) band of $^{14}NO_2$ has just been started.[32] Others have tried to analyze lower resolution spectra of these bands,[4,5] but have not been entirely successful, due largely to the wide spacing of the Q branches of the bands. These authors have tried to explain the large Q-branch spacing as arising from overlapping type-B (perpendicular) bands.

Table V. Vibrational dependence of the rotational constants.

| | $^{14}NO_2$ | $^{15}NO_2$ |
|---|---|---|
| $\alpha_1^A$ | $-0.0724_5 \pm 0.0014$ | $-0.0480_0 \pm 0.0033$ |
| $\alpha_1^B$ | $0.002314 \pm 0.000025$ | $0.002267 \pm 0.000027$ |
| $\alpha_1^C$ | $0.002754 \pm 0.000022$ | $0.002716 \pm 0.000023$ |
| $\alpha_3^A$ | $0.2209_2 \pm 0.0017$ | $0.1868_1 \pm 0.0046$ |
| $\alpha_3^B$ | $0.002753 \pm 0.000030$ | $0.002696 \pm 0.000040$ |
| $\alpha_3^C$ | $0.002732 \pm 0.000030$ | $0.002609 \pm 0.000043$ |

Table VI. Predicted rotational constants for the (0,0,3) and (1,0,3) vibrational levels.

| | $^{14}NO_2$ | $^{15}NO_2$ |
|---|---|---|
| $A_{003}$ | $7.3397_5 \pm 0.0029$ | $7.070_2 \pm 0.008$ |
| $B_{003}$ | $0.42540_6 \pm 0.00005$ | $0.42562_9 \pm 0.00007$ |
| $C_{003}$ | $0.40229_7 \pm 0.00005$ | $0.40166_5 \pm 0.00008$ |
| $A_{103}$ | $7.4122_0 \pm 0.0033$ | $7.118_2 \pm 0.009$ |
| $B_{103}$ | $0.42309_2 \pm 0.00006$ | $0.42336_2 \pm 0.00008$ |
| $C_{103}$ | $0.39954_3 \pm 0.00006$ | $0.39894_9 \pm 0.00008$ |

With the present determination of $\alpha_1^R$ and $\alpha_3^R$, the values of the upper state rotational constants for these bands were calculated and used to predict a spectrum. The calculated rotational constants for the (0,0,3) and (1,0,3) vibrational levels are given in Table VI. The predicted spectra have Q-branch positions which closely match the observed Q branches, showing that the wide Q-branch spacing is due to the relatively large values of $\alpha_3^A$. It should be remarked here that the magnetic rotation spectra have large signals at these Q-branch positions, which also confirms the identification. Thus it appears that only the type-A (0,0,3) and (1,0,3) bands occur in these regions.

## C. SPIN-ROTATION ANALYSIS

### Experimental

Initial spin-splitting measurements were taken from the absorption records. Later, after modifications had been completed on the spectrometer which slightly improved its resolution, new Zeeman records were obtained. The spin-splitting measurements from the zero-field Zeeman runs have been used for the final determinations of the spin-splitting constants.

### (2,0,1) Bands

At least 50 spin-doublets have been identified in each of the (2,0,1) bands. The $\nu^+$ and $\nu^-$ components were assigned by comparing their intensities with the statistical

weights of the levels involved. Of these, 25 $^{14}NO_2$ and 24 $^{15}NO_2$ spin-splittings have been assigned non-zero weights. Equation (27) was first used to fit the $^{14}NO_2$ and $^{15}NO_2$ data separately. The program SPINFIT (see Appendix I) was then modified so that the data from the two molecules could be combined to test the approximation expressed by Eq. (29).

In each case, the fits were first performed holding the ground state effective $\varepsilon$'s at the values which result from the microwave work[3] and then allowing both upper and lower state effective $\varepsilon$'s to vary. The results are summarized in Table VII. The uncertainties on all except the microwave values are 95% simultaneous confidence levels, which in this case are a factor of 2.5 larger than the standard errors of the coefficients as given by the least squares routine.

Comparison of the first and third rows of the table shows that the approximation of Eq. (29) is valid for these data and leads to more accurate values of the $\varepsilon_{201}$ .

Since this determination of the $\varepsilon_{000}$ values does not overlap the values calculated from the microwave work, and the microwave values are generally expected to be far more accurate, the most meaningful results of these fits are probably the values of $(\varepsilon_{201} - \varepsilon_{000})$ given in the third row of Table VII.

In Table VIII are listed the observed and calculated splittings and weights from the fit which led to the effective $\varepsilon$'s in the third row of Table VII.

Table VII. Effective spin-rotation coupling constants for $NO_2$.

| Constants Varied | $^{14}NO_2$ | | | $^{15}NO_2$ | | |
|---|---|---|---|---|---|---|
| | $\epsilon_{000}$ | $\epsilon_{201}$ | $\epsilon_{201}-\epsilon_{000}$ | $\epsilon_{000}$ | $\epsilon_{201}$ | $\epsilon_{201}-\epsilon_{000}$ |
| $^{14}\epsilon_{201}$, $^{15}\epsilon_{201}$ | 0.181644[a] ±0.000002 | 0.1782 ±0.0014[b] | 0.0034 ±0.0014 | 0.173210[a] ±0.000005 | 0.1693 ±0.0016 | 0.0039 ±0.0016 |
| $^{14}\epsilon_{201}$, $^{14}\epsilon_{000}$, $^{15}\epsilon_{201}$, $^{15}\epsilon_{000}$ | 0.1890 ±0.0081 | 0.1857 ±0.0084 | 0.0033 ±0.0008 | 0.1882 ±0.0097 | 0.1832 ±0.0092 | 0.0050 ±0.0009 |
| $\frac{^{14}\epsilon_{201}}{^{14}A_{201}} = \frac{^{15}\epsilon_{201}}{^{15}A_{201}}$ | 0.181644[a] | 0.1781 ±0.0010 | 0.0036 ±0.0010 | 0.173210[a] | 0.1694 ±0.0010 | 0.0038 ±0.0010 |
| $\frac{^{14}\epsilon_{000}}{^{14}A_{000}} = \frac{^{15}\epsilon_{000}}{^{15}A_{000}}$; $\frac{^{14}\epsilon_{201}}{^{14}A_{201}} = \frac{^{15}\epsilon_{201}}{^{15}A_{201}}$ | 0.1916 ±0.0061 | 0.1878 ±0.0060 | 0.00381 ±0.00056 | 0.1827 ±0.0058 | 0.1786 ±0.0057 | 0.00407 ±0.00054 |

[a]Calculated from microwave values of Lees, Curl, and Baker.[3]

[b]95% simultaneous confidence intervals.

Table VIII. (2,0,1) band spin-splittings ($cm^{-1}$).

| | | | $^{14}NO_2$ | | | $^{15}NO_2$ | | |
|---|---|---|---|---|---|---|---|---|
| Branch | $K_{-1}$ | N | OBS | CALC | WT | OBS | CALC | WT |
| P | 1 | 2 | 0.0520 | 0.0579 | 0.1 | | | |
| P | 2 | 3 | 0.1051 | 0.0849 | 0.1 | 0.0930 | 0.0803 | 0.1 |
| P | 2 | 4 | 0.0496 | 0.0443 | 1.0 | | | |
| P | 3 | 4 | 0.1223 | 0.0997 | 0.1 | 0.1027 | 0.0939 | 1.0 |
| P | 3 | 5 | 0.0670 | 0.0610 | 0.1 | 0.0505 | 0.0572 | 0.1 |
| P | 3 | 6 | 0.0424 | 0.0409 | 0.1 | 0.0292 | 0.0383 | 0.2 |
| P | 3 | 7 | | | | 0.0249 | 0.0272 | 0.05 |
| P | 4 | 5 | | | | 0.1081 | 0.1018 | 0.1 |
| P | 4 | 6 | | | | 0.0770 | 0.0680 | 0.1 |
| P | 4 | 7 | | | | 0.0474 | 0.0483 | 0.2 |
| P | 4 | 8 | 0.0360 | 0.0386 | 0.1 | | | |
| P | 5 | 7 | 0.0883 | 0.0809 | 0.1 | 0.0842 | 0.0755 | 0.1 |
| P | 5 | 8 | 0.0644 | 0.0602 | 0.7 | | | |
| P | 5 | 9 | 0.0413 | 0.0463 | 1.0 | 0.0432 | 0.0429 | 0.2 |
| P | 5 | 10 | 0.0313 | 0.0365 | 0.1 | 0.0391 | 0.0337 | 0.1 |
| P | 6 | 12 | 0.0409 | 0.0346 | 0.1 | | | |
| P | 7 | 11 | | | | 0.0463 | 0.0529 | 0.5 |
| P | 7 | 12 | | | | 0.0414 | 0.0431 | 0.3 |
| R | 1 | 1 | -0.0649 | -0.0620 | 1.0 | -0.0714 | -0.0593 | 1.0 |
| R | 2 | 2 | -0.1038 | -0.0949 | 1.0 | -0.1040 | -0.0910 | 1.0 |
| R | 2 | 3 | | | | -0.0490 | -0.0496 | 1.0 |
| R | 2 | 4 | -0.0363 | -0.0329 | 0.1 | -0.0321 | -0.0317 | 0.1 |

Table VIII (Continued)

| | | | $^{14}NO_2$ | | | $^{15}NO_2$ | | |
|---|---|---|---|---|---|---|---|---|
| Branch | $K_{-1}$ | N | OBS | CALC | WT | OBS | CALC | WT |
| R | 3 | 3 | -0.1236 | -0.1161 | 1.0 | | | |
| R | 3 | 4 | -0.0715 | -0.0739 | 1.0 | | | |
| R | 3 | 5 | -0.0464 | -0.0516 | 1.0 | | | |
| R | 3 | 6 | -0.0367 | -0.0383 | 0.2 | -0.0347 | -0.0371 | 0.1 |
| R | 4 | 4 | -0.1271 | -0.1315 | 0.1 | -0.1330 | -0.1266 | 0.1 |
| R | 4 | 5 | | | | -0.0709 | -0.0886 | 0.1 |
| R | 4 | 6 | -0.0551 | -0.0681 | 0.1 | -0.0572 | -0.0659 | 0.1 |
| R | 4 | 7 | -0.0446 | -0.0528 | 0.1 | -0.0548 | -0.0512 | 0.1 |
| R | 4 | 8 | | | | -0.0429 | -0.0411 | 0.1 |
| R | 4 | 9 | | | | -0.0353 | -0.0338 | 0.1 |
| R | 6 | 9 | -0.0800 | -0.0782 | 0.1 | | | |
| R | 6 | 15 | -0.0352 | -0.0334 | 0.2 | | | |
| R | 7 | 18 | -0.0321 | -0.0336 | 0.1 | | | |

## (1,0,1) Bands

The lower energy in the (1,0,1) region, which limits the spectrometer's resolution, and the larger values of (A' - A") for the (1,0,1) bands, which cause a greater overlapping of different K sub-bands, prevent the measurement of many spin-splittings. Only one or two splittings can be assigned non-zero weights out of the ∿40 observed in each band, so a fit has not been attempted.

# D. ZEEMAN SPECTRA

## Experimental Conditions

High resolution Zeeman spectra of the (1,0,1), (2,0,1), and (0,0,3) bands of each molecule were obtained under the same conditions as the absorption spectra (Table II) and with longitudinal magnetic fields of 500, 1000, 2000, 4000, and 6800 gauss.

## Comparison of Experimental Results with Theory

In addition to the transition probabilities given in Eqs. (61), the prediction of the Zeeman spectra requires information about other factors such as the Boltzmann population distribution, the line shape of the Zeeman components, and the slit function shape and half-width.

The population of a rotational level is proportional to

$$N_R = e^{-E(N,K)/kT} \tag{65}$$

where the symmetric top approximation can be used for the rotational energy: $E(N,K) = \bar{B}\, N(N+1) + (A-\bar{B})K^2$, where $\bar{B} = \frac{B+C}{2}$.

The percentage transmission at line center is given by

$$e^{-\alpha N_R |\mu|^2} \times 100 \ , \tag{66}$$

where $|\mu|^2$ is the rotational transition probability and $\alpha$ includes other factors in the line strength such as the pressure dependence, the vibrational transition probability, and the normalization of the population distribution. Since these factors are not all known here, $\alpha$ must be treated as a parameter which is allowed to vary in order to get the best match to the observed spectra. Thus, the percentage absorption at line center is

$$\left(1 - e^{-\alpha N_R |\mu|^2}\right) \times 100 \ . \tag{67}$$

The program PLOTZ (see Appendix I) was written to calculate and plot the percentage absorption as a function of frequency, using ZEMANINT as a subroutine to calculate line positions and transition probabilities for the Zeeman components. Because the slit function is generally larger than the line width, the observed spectra show mainly the shape and width of the slit function. Thus, the line shape of each component can be approximated by a rectangular line shape with height given by Eq. (67) and with a width equal to the minimum plotter unit, which is 0.01 inch or 0.0033

$cm^{-1}$ for the scale of the spectra used here. This is probably not far from the true line width, and any errors are masked by the slit function.

On the basis of the shapes of single lines in the absorption spectra, the slit function is taken to have a Gaussian shape with a half-width at half-intensity of 0.016 $cm^{-1}$.

Figure 8 shows the experimental Zeeman spectra of the band origin region of the (2,0,1) band of $^{14}NO_2$ at fields of 0, 1000, 2000, and 6800 gauss. Figure 9 shows the corresponding theoretical spectra as calculated and plotted by PLOTZ, using $\alpha = 0.07$ . The program finds the apparent percentage absorption as a function of frequency by the following procedure:

(1) The product $N_R|\mu|^2$ and the frequency is calculated for each Zeeman component of each of the lines which are to be plotted. If more than one component occurs within a small frequency interval (which is the minimum plotter unit, or 0.0033 $cm^{-1}$), the values of $N_R|\mu|^2$ in that interval are summed.

(2) The percentage absorption at each point is calculated using Eq. (67).

(3) The specified slit function is used to integrate over the region of interest, giving the predicted spectrum. The zero-field asymmetric top frequencies used for the transitions are those calculated from the constants given for

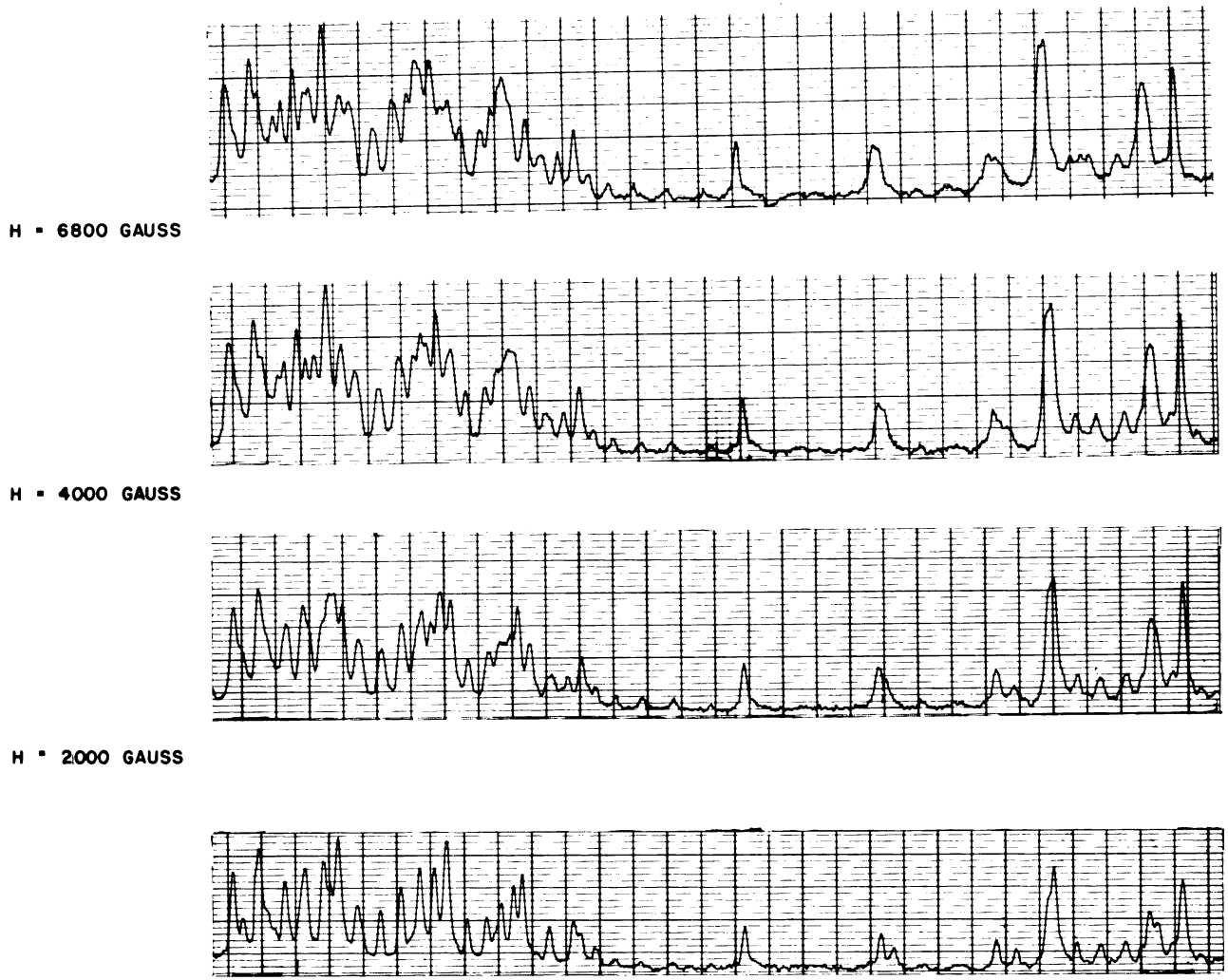



Fig. 8. Experimental Zeeman spectra for the band origin region of the (2,0,1) band of $^{14}NO_2$.

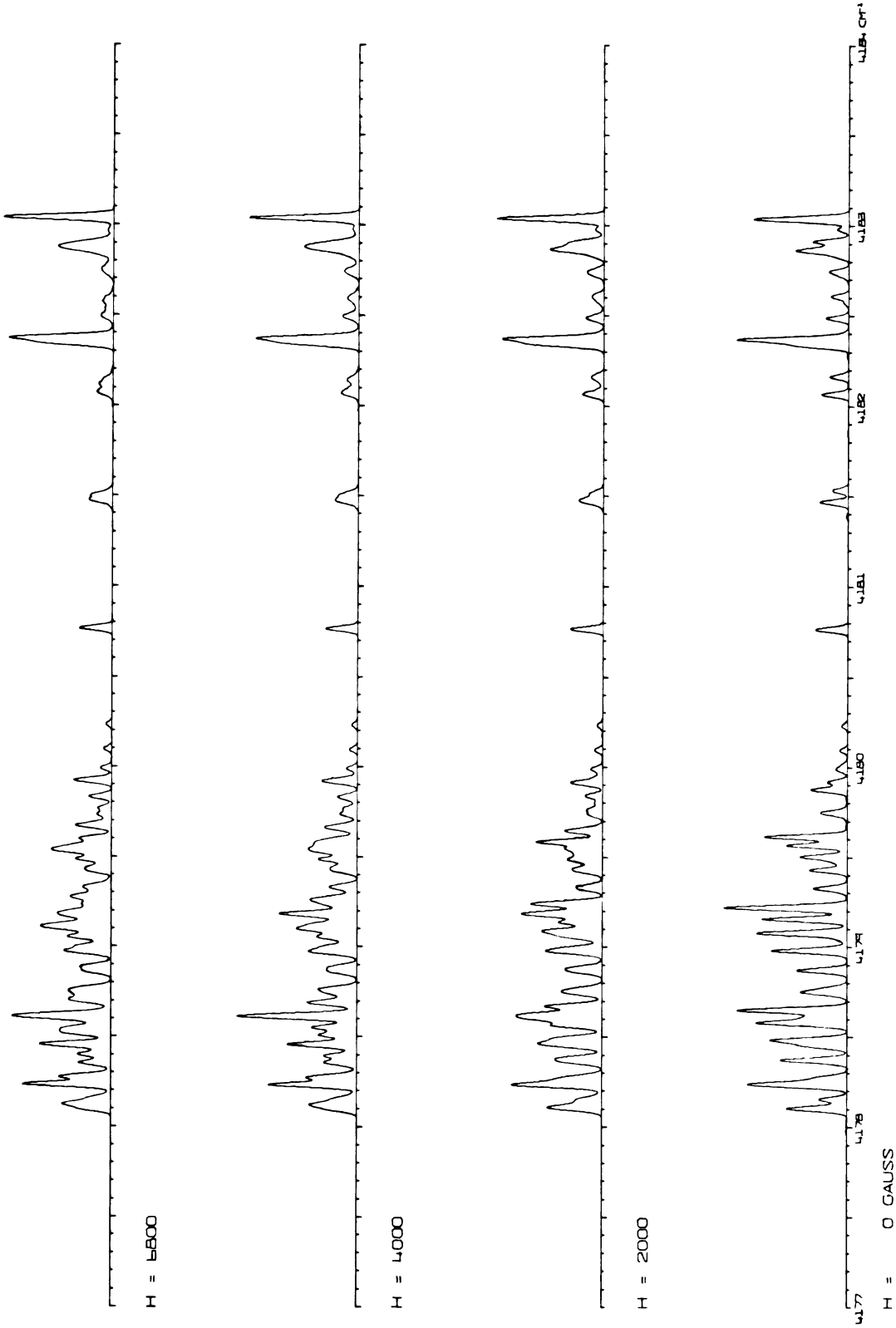



Fig. 9. Predicted Zeeman spectra for the band origin region of the (2,0,1) band of $^{14}NO_2$.

this band in Table IV. The strongest line plotted at zero field corresponds to ∿35% absorption.

Varying α has little effect on the relative intensities of the different rotational transitions and very little effect on the Zeeman structure of a given rotational transition. The value of α used is found to give the best overall match between the observed and theoretical intensities.

## E. MAGNETIC ROTATION SPECTRA

### Experimental

Magnetic rotation spectra at various fields were obtained for each of the bands studied. Figure 10 shows slave-recorder tracings of the magnetic rotation spectra of the (1,0,1) band of $^{14}NO_2$. The P-branch region (below 2890 $cm^{-1}$) was run at a field of 3500 gauss, and the Q-branch region at 2500 gauss. The strongest signals are from $Q_K(N)$ transitions with K = 4 through 9. The P-branch signals come from $P_K(N)$ transitions with K = 6 and 7 and N = 13 through 24.

### Analysis

The strongest magnetic rotation signals invariably come from the Q-branch transitions. The signals from the Q branch for a given K increase as the field is increased until a certain field is reached, after which they decrease. The field at which a Q branch gives the maximum signal varies with the value of K for the branch. Study of the

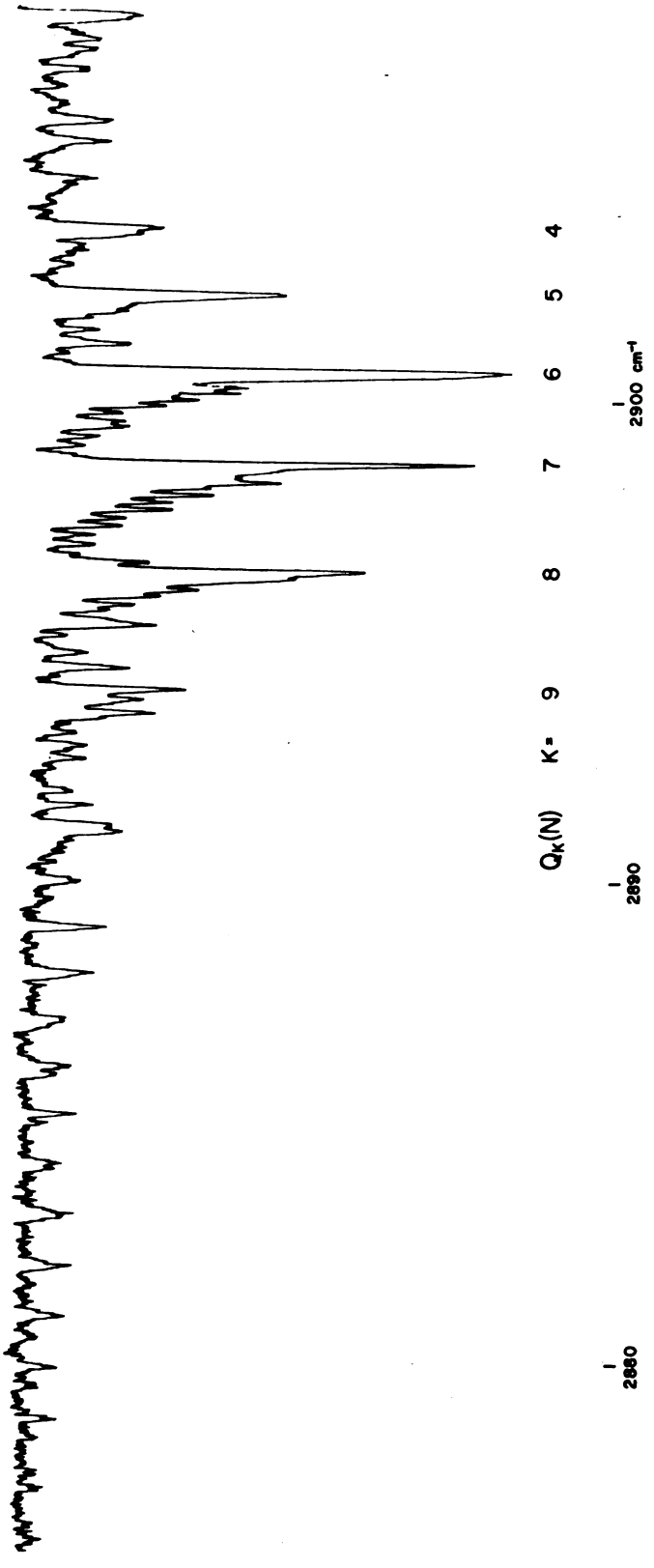



Fig. 10. Magnetic rotation spectrum of the (1,0,1) band of $^{14}NO_2$. The P-branch region (below 2890 $cm^{-1}$) was run at 3500 gauss, and the Q-branch at 2500 gauss.

variations of the Zeeman patterns of a Q-branch transition indicates that there is a field strength at which the $\Delta M_N$=+1 transitions from the two components of the spin-doublet superimpose. Thus, at this field there is a strongly absorbing region of $\Delta M_N$=+1 transitions at line center, with weaker $\Delta M_N$=-1 absorption in the wings of the line. For each Q branch this is the field for which the magnetic rotation signals are the strongest. For the $Q_7(7)$ transition shown in Fig. 7 this occurs at a field strength near 2000 gauss.

The fact that the field at which this maximum signal occurs is found, experimentally, to depend on K can be attributed to the fact that the zero-field separation of the spin-doublets varies as $K^2$. At low K values, a smaller field will move the $\Delta M_N$=+1 components to superposition, while at high K values, the field must be considerably stronger. If the field is increased above the point of strongest signal, the $\Delta M_N$=+1 and $\Delta M_N$=-1 transitions move closer to one another, as shown in Fig. 7, until at high fields there is so much overlapping that little magnetic rotation signal can be expected. Experimentally, as the field is increased, the signal decreases until at the maximum field (6800 gauss) there is essentially no magnetic rotation spectrum. Calculation of the index of refraction and absorption coefficient curves for right and left circularly polarized light at the various fields should show maximum differences corresponding to the fields at which maximum signals are found, and small differences at higher fields.

As shown in Fig. 6, the Zeeman patterns for P-branch lines are not the same as the Q-branch patterns. As the field is applied, the stronger components tend to remain near their field-free positions so that there is never a grouping of strong $\Delta M_N=+1$ or $\Delta M_N=-1$ transitions in a single region, as there is for the Q-branch lines. This explains the weaker signals which are found in the P branch. The only R-branch signals appear to come from low N transitions near the band origin. The lack of further signals from R-branch lines, which have Zeeman patterns similar to those of the P branch, is probably due to the great amount of overlapping of transitions which would tend to cancel Faraday rotation and circular dichroism effects.

The strongest P-branch signals for the (2,0,1) band of $^{14}NO_2$ come from the K=5 series with N = 8 to 12, at a field of 2000 gauss. From this it appears that the strongest P-branch signals are to be expected from lines whose spin-doublet is just resolved (0.03-0.04 $cm^{-1}$) so that in the region between the doublet components the monochromator passes a band of frequencies for which there has been predominantly $\Delta M_N=+1$ (or -1) absorption.

From the Zeeman patterns shown in Figs. 6 and 7 it appears that the observed magnetic rotation signals have contributions from both Faraday rotation and circular dichroism. Thus, a complete explanation of the experimental spectra will require a detailed quantitative analysis.

Strong magnetic rotation signals were obtained from what are here identified as the Q branches of the type-A (0,0,3) bands of $^{14}NO_2$ and $^{15}NO_2$. No signals could be obtained from the weak (0,0,2) type-B bands. This supports the conclusion reached in Section B of this chapter that the signals, and thus the Q branches found in the (0,0,3) region, must come from the type-A (0,0,3) band and not from an underlying type-B band.

## SUMMARY

Analysis of infrared ground state combination differences combined with microwave transition frequencies has led to the determination of more accurate estimates of the ground state molecular constants of $^{14}NO_2$ and $^{15}NO_2$, including empirical $P^6$ terms. Accurate upper state rotational and centrifugal distortion constants and band origins have been obtained for the (1,0,1) and (2,0,1) bands of $^{14}NO_2$ and $^{15}NO_2$. In addition, the change in the effective spin-rotation coupling constant between the ground and the (2,0,1) vibrational states has been determined for each isotopic species.

Theoretical expressions have been found which give the frequencies and transition probabilities for the Zeeman components of absorption transitions at all magnetic fields. The spectra predicted by these expressions match very closely the details of the experimental spectra at all magnetic fields available. Use of these expressions should lead to a quantitative explanation of the observed magnetic rotation spectra.

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17. The routine used to calculate asymmetric rotor energies was furnished by J. Hand, Chemistry Department, Michigan State University.
18. The Hydel system was originally used to digitize cloud chamber data. Professor T. H. Edwards recognized its usefulness for reduction of spectroscopic data and developed the photographic method for converting our data to 35 mm film frames. The system can reproduce measurements to better than 0.03 mm on the original charts, which corresponds to 0.0002 to 0.0008 $cm^{-1}$, depending on the dispersion, chart speed, fringe order, etc. The Hydel system is described briefly by T. L. Barnett, Thesis, Michigan State University (1967).
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# APPENDIX I

## COMPUTER PROGRAMS WRITTEN

Many computer programs were written in the course of the work described in this thesis. The most important of these are described below. All least squares sections are based on a routine written by M. A. Efroymson[33] of Esso Research and Engineering Company, and the calculations of the asymmetric rotor energies are based on a program written by J. Hand[17] while at Michigan State University.

### A. SCAN

This program converts digitized data from the Hydel system[18] into the fringe positions and frequencies of the absorption lines as recorded on the chart.

Error flags are printed out if the fringe spacing varies by more than 10%, if the rotation angle is greater than $\pm 0.005$ radians, or if any of the rotation card data points is off by more than 10 microns on the film.

Since the use of the Hydel system and SCAN to reduce data is now a standard procedure in this laboratory, it is not necessary to provide a description of the program here.

A listing of the program SCAN follows.

```
      PROGRAM SCAN
      DIMENSIONXM(6),YM(6),FRNGX(100),PSEP(100),FGSEP(100),I1(2),I2(2),
     1IHEAD(9),NAME(2 ),NHEAD(10),DELX(6),IPFR(3),IPEN(2)
      DATA(IPEN=8H6FIRST  ,8H6SECOND )
    4 PRINT 9701
      READ 7,NAME,IFDONE
    7 FORMAT (2A8,56X,A8)
      IF(IFDONE-8HNEW SCAN)5,6
    5 IF(IFDONE-8HOLD SCAN) 8,9
    8 PRINT 10
   10 FORMAT (*-NO NAME CARD * - - ABORT*)
      GO TO 102
    9 INEW=0
      GO TO 1
    6 INEW=1
    1 READ 3, IHEAD,IFDONE
      PRINT 3, IHEAD
      IF(IFDONE-8HEND HEAD) 1,2
    2 NFRM=NCAL=IP=0
      NIP=IH=1
      XFSEP=FSEP=0.0
      ASSIGN 3600 TO NGO
  101 READ 100, (XM(I), YM(I), I =1,6), ICODE,IFR
      IF(ICODE-6) 202,200,203
  203 IF(ICODE-8) 7000,4,102
  202 IF(4-ICODE)5010,4000,204
  204 IF(ICODE-2) 209,2000,200
  205 IF(-ICODE) 1000,105,105
  105 PRINT 106,(XM(I),YM(I),I=1,6)
      GO TO 101
  102 PRINT 9701$STOP
  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 XFRM=XM
      XFRNG=YM
      FRNG=XFRNG-1.0
      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(ABSF(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
     2ICRONS*/* 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
      PSEPSUM = 0
      DO 3701 J=1,IP
 3701 PSEPSUM=PSEPSUM+PSEP(J)
      PENSEP = PSEPSUM/ IP
      PRINT9300,PENSEP
      GO TO 32
 4000 NCAL=1
      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
      PRINT 9400, A, B
      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(ABSF(FGSEP(I)-FGSEP(I-1)) .GT. AVESEP) IBAD = 1
     IF(IBAD) PRINT 6208
     M=0
     IF(NCAL) PRINT 9650,A,B
     PRINT 9655
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 FRNO1=FRNG+L+(XIR-FRNGX(L))/FGSEP(L+1)
     IF(.NOT.NCAL) GO TO 9000
     FREQ1=A+B*FRNO1
     PRINT 9651,NEXT,FRNO1,FREQ1
     GO TO 6001
9000 PRINT 9651,NEXT,FRNO1
6001 CONTINUE
     GO TO 101
7000 READ3,NHEADSPRINT3,NHEADSGOTO101
   3 FORMAT (10A8)
 100 FORMAT (6(2F5.X),I1,A4)
 106 FORMAT (*0THIS CARD HAS A BLANK OR ZERO CODE*  5X6(2F5.X)  /)
6208 FORMAT (***80X*FRINGE SPACING VARIATION .GT. 10%*)
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*      B =*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,F15,4)
9655 FORMAT (*0*9X*FRINGE NUMBER   FREQUENCY*)
9701 FORMAT (*5*/*1*9A8)
     END
```

## B. CALFIT

This is a least squares routine specialized to fit the fringe numbers of calibration lines to their known frequencies using the formula, (frequency) = A + B·(fringe number). The values of A and B are input to SCAN to allow it to convert observed fringe numbers to frequencies. If the worst data point is off more than 0.005 $cm^{-1}$, it is deleted, and the fit is repeated. This process will be repeated until up to five data points have been deleted.

### STRUCTURE OF DATA DECK

| Card Type | Format | Columns | Information |
|---|---|---|---|
| 1 | 10A8 | 1-80 | Heading cards to be printed out. The last one must have "END HEAD" in columns 73-80. |
| Data cards (up to 500) | | | |
| 2 | 3F15 | 1-15 | Known calibration frequency. |
| | | 16-30 | Observed fringe number. |
| | | 31-45 | Assigned weight. |
| 3 | A8 | 73-80 | "END DATA" to signal end of data. |
| 4 | Start new set of data with another card type 1, or blank card to stop execution. | | |

## C. CDSORT

This program inputs and stores all of the identified transition frequencies of a given band. It forms frequency differences for those transitions having common upper or lower quantum numbers and stores these differences as

weighted GSCD or USCD. The differences are also printed out along with the frequencies of the lines involved. After all such differences have been found and averaged, the resulting set of USCD are output as punched cards ready for input to CDFIT.

Transitions for the next band of the same molecule are then input, and the above is repeated, with the new GSCD being averaged with those of the first band. After all of the desired bands have been processed, the resulting set of averaged, weighted GSCD is output.

STRUCTURE OF DATA DECK

| Card Type | Format | Columns | Information |
|---|---|---|---|
| 1 | I5 | 1-5 | 1, 2, or 3 will request program to find GSCD, USCD, or both. |
| | A8 | 6-13 | Molecule [e.g., "14NO2"]. |
| | A8 | 14-21 | Band [e.g., "(2,0,1)"]. |
| 2 | (X,6I3,F15,F13) | | Identified transitions for this band. The format is identical to that used for SPECFIT data. |
| 3 | A8 | 73-80 | "END DATA" signals end of data. |
| 4 | Card types 1-3 for the next band of this molecule, or blank card to signal that last band of this molecule has been input so that averaged GSCD will be output. | | |
| 5 | Card type 1 for new molecule, or blank card to stop. | | |

A listing of the program CDSORT follows.

```
      PROGRAM CDSORT
      COMMON J(2000,2),JJ(6),FREQ(2000),WHT(2000),KK(630,2,2),
     1CDIFF(630,2),CDWT(630,2)
      DIMENSION IH(2)
      DATA (IH=8H GROUND ,8H  UPPER )
    1 READ 10,IS,MOL,IHEAD,TOL
      IF(.NOT. TOL) TOL=0.01
      IF(IS) 4,5
    5 IHEAD = 8HAVERAGE
      IF(NSTOP) STOP
      NSTOP=I=1
      MOL=IMOL
      GO TO 220
    4 N=NSTOP=0
      IMOL=MOL
    7 N=N+1
    9 READ 101,JJ,FREQ(N),WHT(N),IDENT
      IF(IDENT=8HEND DATA) 6,8
    6 IF(FREQ(N) .LE. 100.0) GO TO 9
      ENCODE (8,11,J(N,1)) JJ(1),JJ(2),JJ(3)
      ENCODE (8,11,J(N,2)) JJ(4),JJ(5),JJ(6)
      GO TO 7
    8 NODATA=N-1
   21 GO TO (1,22,23,24),IS+1
   22 I=1
      I1=2
      IS=0
      GO TO 25
   23 I=2
      I1=1
      IS=0
      GO TO 25
   24 I=1
      IS=I1=2
   25 PRINT 2,MOL,IHEAD,IH(I),NODATA
      NCD=0
      DO 111 M=1,NODATA
      M1=M+1
      DO 111 N=M1,NODATA
      IF(J(N,I) .NE. J(M,I)) GO TO 111
      CD=FREQ(N)-FREQ(M)
      MM=M
      NN=N
      IF(CD) 118,111,117
  118 MM=N
      NN=M
      CD=-CD
  117 GO TO (311,312),I
  311 N1=MM$N2=NN$GO TO 313
  312 N1=NN$N2=MM
  313 DECODE (8,11,J(N1,I1)) JJ(1),JJ(2),JJ(3)
      DECODE (8,11,J(N2,I1)) JJ(4),JJ(5),JJ(6)
      FM=FREQ(MM)
      FN=FREQ(NN)
```

```
      WN=WHT(NN)
      WM=WHT(MM)
      WT=2.0*WN*WM/(WN*WM*0.0001)
      PRINT121,JJ,CD,WT,(J(NN,K),K=1,2),FN,WN,(J(MM,K),K=1,2),FM,WM
      IF(JJ(2).LE.8) IF(WT)122,111
      PRINT 55
      GO TO 111
  122 NCD=NCD+1
      NM=70*JJ(2)+JJ(1)+20
      IF(JJ(1)+JJ(4)-2) NM=NM+20
      IF(CDWT(NM,I)) 201,203
  201 A=CDWT(NM,I)+WT
      IF(ABSF(CD-CDIFF(NM,I)) .GT. TOL) PRINT 204,TOL
      CDIFF(NM,I)=(CDIFF(NM,I)*CDWT(NM,I)*CD*WT)/A
      CDWT(NM,I)=A
      GO TO 111
  203 CDIFF(NM,I)=CD
      CDWT(NM,I)=WT
      KK(NM,1,I)=J(N1,I1)
      KK(NM,2,I)=J(N2,I1)
  111 CONTINUE
      PRINT3,NCD
      GO TO (21,220),I
  220 NPUNCH=0
      PRINT 2
      DO 211 K=1,9
      KM=70*K+1
      DO 211 M=1,70
      MN=KM-M
      CDWHT=CDWT(MN,I)
      IF(CDWHT) 213,211
  213 J1=KK(MN,1,I)
      J2=KK(MN,2,I)
      CD=CDIFF(MN,I)
      PRINT 100,J1,J2,CD,CDWHT
      PUNCH 100,J1,J2,CD,CDWHT
      NPUNCH=NPUNCH+1
  211 CDWT(MN,I)=0.0
      PUNCH 124
      PRINT125,NPUNCH,MOL,IH(I)
      GO TO (1,21),I
    2 FORMAT(*1*3A8*STATE COMBINATION DIFFERENCES FROM*I4* FREQUENCIES*/
     1/3(2(*    J K= K**)14X*WHT*5X)/***21X*COMB DIFF*2(33X*FREQUENCY*)/)
    3 FORMAT(*7*I4* COMBINATION DIFFERENCES WITH NON-ZERO WEIGHTS*)
   10 FORMAT (I5,2A8,F10)
   11 FORMAT (I2,X,I2,X,I2)
   55 FORMAT (***122X*K .GT. 8*)
  100 FORMAT(2XA8,XA8,F15.4,F13.2)
  101 FORMAT (X6I3,F15,F13.25XA8)
  121 FORMAT (2(X3I3),F11.4,F6.2,2(5X,2A10,F11.4,F6.2))
  124 FORMAT (72X*END DATA*)
  125 FORMAT(*7PUNCHED*I4* AVERAGE*A9,R7*STATE COMBINATION DIFFERENCES*)
  204 FORMAT (***122X*DIFF GT*F6.3)
      END
```

## D. CDFIT

Built around the asymmetric rotor energy level routine[17] and the least squares routine,[32] this program generates a set of calculated energy levels, along with values of $\zeta$, $\xi$, and $\eta$, from a set of trial constants. Observed combination differences are then read in and compared with combination differences formed from the calculated energies. The set of observed minus calculated combination differences are fit by the least squares section to determine corrections to the trial values of the constants [cf. Eq. (17)]. The particular set of constants which is allowed to vary in a given fit is specified on a parameter card. After the fit the deviation (times the square root of the weight) of the worst data point is compared with an input tolerance, and if the tolerance is exceeded, the data point is given a zero weight, and the fit is repeated. Another input tolerance specifies how many times this process will be repeated.

Any number of parameter cards can be read in. This allows the determination of corrections for several different sets of variables. For each parameter card, all weights are reset to their initial values so that deleted points will be included again.

STRUCTURE OF DATA DECK

| Card Type | Format | Columns | Information |
|---|---|---|---|
| 1 | I5 | 1-5 | Maximum value of N ($\leq$48) contained in input data if fitting GSCD. |
| | I5 | 6-10 | Maximum value of N ($\leq$48) contained in input data if fitting USCD. |
| | F10 | 11-20 | If "observed minus calculated" is larger than this number, the data point is deleted on input. (Set to 10.0 if left blank.) |
| | 2A8 | 21-36 | Identification of combination differences fitted [e.g., "(2,0,1)-(1,0,1)"]. |
| | A8 | 37-44 | Molecule [e.g., "14NO2"]. |
| Trial constants (three cards for GSCD; four cards for USCD) | | | |
| 2a | 3F15 | 1-45 | Values of A, B, and C for ground state: this card is needed only when fitting USCD. |
| 2b | 3F15 | 1-45 | A, B, C. |
| 3 | 4F15 | 1-60 | $\tau_1$, $\tau_2$, $\tau_3$, $\tau_4$. |
| 4 | 4F15 | 1-60 | $H_N$, $H_{NK}$, $H_{KN}$, $H_K$. |
| Data (one card for each observed combination difference; up to 300 data points may be input) | | | |
| 5 | 6I3 | 2-19 | Values of N, $K_{-1}$, $K_{+1}$ for upper and lower rotational level, respectively. |
| | F20 | 20-39 | Observed combination difference. |
| | F10 | 40-49 | Weight assigned to this observation. |
| 6 | A8 | 73-80 | "END DATA" signals end of data. |
| Parameter cards (one card for each set of constants to be varied) | | | |
| 7 | 13I1 | 1-13 | Non-zero numbers in any of these columns will enter the corresponding constants in the fit. The 13 constants are (B+C)/2, (B-C)/2, A, $\tau_1$, |

| Card Type | Format | Columns | Information |
|---|---|---|---|
| | | | $\tau_2$, $\tau_3$, $\tau_4$, $H_N$, $H_{NK}$, $H_{KN}$, $H_K$, B, and C. |
| | F10 | 21-30 | This number gives the minimum value a variable's diagonal element in the least squares matrix can have if the variable is to be entered. If left blank, it is set to 0.0001. |
| | I2 | 49-50 | A non-zero number will cause all of the least squares steps to be printed out. If left blank, only the final coefficients and standard errors for each fit will be printed out. |
| | I5 | 60-65 | Maximum number of data points to be deleted after the initial fit. |
| | F5 | 66-70 | Tolerance for deleting data points after the initial fit. |
| | A8 | 73-80 | "END HEAD." Otherwise will read and print succeeding cards until "END HEAD" is encountered in columns 73-80. |
| 8 | A8 | 73-80 | "LAST FIT" signals end of execution. |

A listing of the program CDFIT follows.

```
      PROGRAM C D FIT
      DIMENSION I1(13),I2(12),I3(2),I5(3),NVARY(11)
      DATA(I1=7H(B+C)/2,7H(B-C)/2,1HA,5HTAAAA,5HTBBBB,5HTAABB,5HTABAB,2H
     1HN,3HHNK,3HHKN,2HHK,1HB,1HC,3H  A,3H  B,3H  C,5HKAPPA,5HTAAAA,5HTB
     1BBB,5HTAABB,5HTABAB,3H HN,4H HNK,4H HKN,3H HK,7H GROUND,7H  UPPER)
      COMMON /1/ OLDCNST(12)
      EQUIVALENCE(OLDCNST(1),A),(OLDCNST(2),B),(OLDCNST(3),C),(OLDCNST(4
     1),CAPPA)
      COMMON/2/E(48,16,25),DATA(14,500),VECTOR(15,15),INDEX(14),SIGMA(14
     1),COEN(14),SIGMCO(14),NK(13),NUSE(500),CORR(13),ADD(12),CNST(12),
     2IH(10),N1(13),NOTIN(13)
      EQUIVALENCE(E,DATA),(E(7001),VECTOR),(E(7226),INDEX),(E(7240),SIGM
     1A),(E(7254),COEN),(E(7268),SIGMCO),(E(7282),NK),(E(7295),NUSE),
     2(E(7795),CORR),(E(7810),ADD),(E(7825),CNST),(E(7840),IH),(E(7850),
     3N1),(E(7863),NOTIN)
      COMMON/3/WT(300),D(50),T(25),TT(25),R(25),HH(25),PIK(25),PIKJ(25),
     1PIKK(25)
      EQUIVALENCE (WT,D),(WT(51),T),(WT(76),TT),(WT(101),R),(WT(126),HH)
     1,(WT(151),PIK),(WT(176),PIKJ),(WT(201),PIKK)
      COMMON/4/H(25,25),JK(2,300)
      EQUIVALENCE (H,JK)
      COMMON/5/OBS(300),CALC(300),CONST(13,300),NDENT(300),KKJ(6),
     1Z(11,2),ENG(2)
    1 READ 9000,NMAXG,NMAXU,CDEVMAX,I5
      IF(NMAXG) 3,4
    3 NS=1
      NC=5
      NMAX=NMAXG
      GOTO6
    2 STOP
    4 IF(,NOT,NMAXU) GO TO 2
      NS=2
      NC=1
      NMAX=NMAXU
    6 READ 701, A,B,C
      RR=(C/A)**2
      SS=(C/B)**2
      READ 701,(OLDCNST(I),I=NC,12)
      IF(NMAX,GT,48) NMAX=48
      IF( ,NOT, CDEVMAX) CDEVMAX=10.0
      CAPPA=(2.*B-A-C)/(A-C)
      IF(CAPPA)7,7,8
    8 BP=(CAPPA-1.0)/(CAPPA+3.0)
      BC=0.5*(A+B)
      ABC=C-BC
      L1=3
      L2=MM2=1
      L3=MM1=2
      I1(1)=7H(A+B)/2SI1(2)=7H(A-B)/2SI1(3)=1HCSI1(12)=1HA $ I1(13)=1HB
      GO TO 9
    7 BP=(CAPPA+1.0)/(CAPPA-3.0)
      BC=0.5*(B+C)
      ABC=A-BC
      L1=MM1=1
```

```
      L2=MM2+2
      L3=3
      I1(1)=7H(B+C)/2$I1(2)=7H(B-C)/2$I1(3)=1HA$I1(12)=1HB $ I1(13)=1HC
     9 E(1,6)=E(1,7)=E(1,10)=E(1,11)=E(1,14)=E(1,15)=E(2,6)=E(2,7)=E(2,10
       1)=E(2,11)=E(2,14)=E(2,15)=1.$E(2,12)=E(3,12)=16.0$E(2,16)=E(3,16)=
       264.$E=E(1,5)=E(1,9)=E(1,13)=.0$E(2,4)=E(2,8)=E(3,4)=E(3,8)=4.
      BP2=BP*BP
      E(1,3)=1.-BP
      E(1,2)=1.+BP
      E(2)=2.-SQRTF(4.+12.*BP2)
      E(2,1,2)=4.-E(2)
      E(2,3)=1.-3.*BP
      E(2,2)=-E(2,3)+2.0
      E(3,3,1)=5.-3.*BP-SQRTF(16.+24.*BP+24.*BP2)
      E(3,3,2)=10.+6.*BP-E(3,3)
      E(3,2,1)=5.+3.*BP-SQRTF(16.-24.*BP+24.*BP2)
      E(3,2,2)=10.+6.*BP-E(3,2)
      E(3,1,1)=2.-SQRTF(4.+60.*BP2)
      E(3,1,2)=4.-E(3)
      DO139J=2,NMAX
      LLAST=0
      IDENT=1
      XJ=J
      AJPLS=XJ*XJ+XJ
      ABS=AJPLS*BP+0.5
      DO 14 I=1,J
      XI=I+I
   14 D(I)=0.5+BP+SQRTF((AJPLS-XI)**2-XI)
      D(1)=1.41421356241*D(1)
   20 L=0.5*(XJ+2.0)
      DO 26 I=1,L
      IP3=I+3
      DO 26 IJ=1,L
      H(I,IJ)=0.
      GOTO(26,24,23,25,26),(IP3-IJ)
   23 H(I,I) = (I+I-2)**2
      GOTO 26
   24 H(I,IJ)=D(I+I-1)
      GOTO 26
   25 H(I,IJ)=H(IJ,I)
   26 CONTINUE
      GO TO 53
   27 L=0.5*(XJ+1.0)
      DO 35 I=1,L
      IK=I+I
      IP3=I+3
      DO 35 IJ=1,L
      H(I,IJ)=0.
      GOTO(35,31,32,30,35),(IP3-IJ)
   30 H(I,IJ)=H(IJ,I)
      GOTO 35
   31 H(I,IJ)=D(IK)
      GOTO 35
   32 GOTO(33,34),I
```

```
33 H=1.*ARS
   GOTO 35
34 H(I,I) = (IK-1)**2
35 CONTINUE
   GO TO 53
36 L=0.5*(XJ+1.0)
   DO 44 I=1,L
   IK=I+I
   IP3=I+3
   DO 441J=1,L
   H(I,IJ)=0.
   GOTO(44,40,41,39,44),(IP3-IJ)
39 H(I,IJ)=H(IJ,I)
   GOTO 44
40 H(I,IJ)=D(IK)
   GOTO 44
41 GOTO(42,43),I
42 H=1.*ARS
   GOTO 44
43 H(I,I) = (IK-1)**2
44 CONTINUE
   GO TO 53
45 L=0.5*XJ
   DO 51  I=1,L
   IP3=I+3
   DO 51 IJ=1,L
   H(I,IJ)=0.
   GOTO(51,49,50,48,51),(IP3-IJ)
48 H(I,IJ)=H(IJ,I)
   GOTO 51
49 H(I,IJ)=D(I+I+1)
   GOTO 51
50 H(I,I) = 4*I*I
51 CONTINUE
53 CONTINUE
   LK=L-1
   GOTO(130,54),L
54 DO 128 K=1,L
   IF(J-3)60,60,55
55 IF(K-LK)56,56,58
56 E(J,IDENT,K)=2.*E(J-1,IDENT,K)-E(J-2,IDENT,K)
   GOTO 60
58 TUM=0.0SSUM=H(L,L)
   DO 59 IJ=1,LK
   SUM=SUM+H(IJ,IJ)
59 TUM=TUM+E(J,IDENT,IJ)
   E(J,IDENT,L)=SUM-TUM
60 LOOP=LOOP2=K
   LOOP1=1
   LOOP3=0
   FUNTEST=5.E-7
61 LIN=L-LOOP
   LIM = LIN - 2
   KJ=LOOP-1
```

```
      KL=LOOP+1
      R=E(J,IDENT,K)-H
      GOTO(64,62),LOOP
   62 HH = H(1,2)*H(1,2)
      DO 63 I=2,KJ
      HH(I) = H(I,I+1)*H(I,I+1)
   63 R(I)=E(J,IDENT,K)-H(I,I)-HH(I-1)/R(I-1)
   64 R(L)=E(J,IDENT,K)-H(L,L)
      GOTO(67,65),LIN
   65 HH(L) = H(L,L-1)*H(L,L-1)
      DO 66 I=1,LIM
      LI=L-I
      HH(LI) = H(LI,LI+1)*H(LI,LI+1)
   66 R(LI)=E(J,IDENT,K)-H(LI,LI)-HH(LI+1)/R(LI+1)
      R(KL)=E(J,IDENT,K)-H(KL,KL)-HH(KL+1)/R(KL+1)
   67 HH(KL) = H(KL,KL+1)*H(KL,KL-1)
   68 IF(LOOP1-1)69,70
   69 IF (LOOP1-10) 92,92,70
   70 IF(LOOP-L)71,74
   71 DO 72 I=KL,L
   72 TT(I)=H(I,I-1)/R(I)
      T(LOOP)=1.
      DO 73 I=KL,L
   73 T(I)=TT(I)*T(I-1)
   74 IF(LOOP-1)75,78
   75 DO 76 I=1,KJ
   76 TT(I)=H(I,I+1)/R(I)
      T(LOOP)=1.
      DO 77 I=1,KJ
   77 T(LOOP-I)=TT(LOOP-I)*T(LOOP-I+1)
   78 DFUNCT=0.0
      DO 79 I=1,L
   79 DFUNCT=DFUNCT+T(I)*T(I)
      SUM=1./SQRTF(DFUNCT)
      DO 80 I=1,L
   80 T(I)=T(I)*SUM
      IF(LOOP1-1)81,82
   81 IF(LOOP1-11)92,82
   82 ITTY=1
   83 I=1
   84 IF(I+ITTY-L)85,85,88
   85 TEST = T(ITTY)*T(ITTY) - T(ITTY+I)*T(ITTY+I)
      IF(TEST)86,87,87
   86 ITTY=ITTY+I
      GOTO 83
   87 I=I+1
      GOTO 84
   88 LOOP=ITTY
      IF(LOOP-LOOP2)89,92
   89 IF(LOOP1-11)90,91
   90 LOOP1=LOOP1+1
      GOTO 61
   91 LOOP2=LOOP
      LOOP1=11
```

```
      GOTO 61
   92 IF(LOOP1-12)93,110,110
   93 IF(LOOP-1)94,95
   94 IF(LOOP-L)99,97
   95 FUNCT=E(J,IDENT,K)-H(LOOP,LOOP)-HH(KL)/R(KL)
      PROD=1.
      DO 96 I=1,LK
      IJ=L-I+1
   96 PROD = 1. + PROD*HH(IJ)/R(IJ)/R(IJ)
      DFUNCT=PROD
      GOTO 102
   97 FUNCT=E(J,IDENT,K)-H(LOOP,LOOP)-HH(KJ)/R(KJ)
      PROD=1.
      DO 98 I=1,LK
   98 PROD = 1. + PROD*HH(I)/R(I)/R(I)
      DFUNCT=PROD
      GOTO 102
   99 FUNCT=E(J,IDENT,K)-H(LOOP,LOOP)-HH(KL)/R(KL)-HH(KJ)/R(KJ)
      PROD=1.
      DO 100 I=1,KJ
  100 PROD = 1. + PROD*HH(I)/R(I)/R(I)
      DFUNCT=PROD-1.
      PROD=1.
      DO 101 I=1,LIN
      IJ=L-I+1
  101 PROD = 1. + PROD*HH(IJ)/R(IJ)/R(IJ)
      DFUNCT=DFUNCT+PROD
  102 LOOP2=LOOP
      LOOP1=LOOP1+1
      LOOP3=LOOP3+1
      IF(FUNTEST-ABSF(FUNCT))106,106,104
  104 IF(LOOP1-12)105,108,110
  105 LOOP1=11
      GOTO 108
  106 IF(LOOP3-10)108,109,109
  108 E(J,IDENT,K)=E(J,IDENT,K)-FUNCT/DFUNCT
      GOTO 61
  109 PRINT 702
      GOTO 128
  110 CONTINUE
      DO114I=1,L
      GOTO(113,115,115,117),IDENT
  113 PIK(I)=(I+I-2)**2
      GOTO116
  115 PIK(I)=(I+I-1)**2
      GOTO116
  117 PIK(I)=4*I*I
  116 PIKK(I)=PIK(I)*PIK(I)
  114 PIKJ(I) = PIKK(I)*PIK(I)
  119 IJK=1$ITOP=LK$IF(LOOP-1)120,132
  120 IF(LOOP-L)125,134
  134 E(J,IDENT+12,K)=PROE/DFUNCT
      E(J,IDENT+8,K)=PROC/DFUNCT
      E(J,IDENT+4,K)=PROD/DFUNCT
```

```
      GOTO 128
  129 ITOP=KJ=LOOP+1$IJK=2
      KL=LOOP+1
      LIN=L-LOOP
  134 PROE=PIKJ
      PROC=PIKK
      PROD=PIK
      DO126I=1,ITOP
      HHRR=HH(I)/R(I)/R(I)
      PROE = PIKJ(I+1) + PROE*HHRR
      PROC = PIKK(I+1) + PROC*HHRR
  126 PROD = PIK (I+1) + PROD*HHRR
      GOTO(131,135),IJK
  135 E(J,IDENT+12,K)=PROE
      E(J,IDENT+8,K)=PROC
      E(J,IDENT+4,K)=PROD
      ITOP=LIN
  132 PROC=PIKK(L)
      PROE=PIKJ(L)
      PROD=PIK(L)
      DO 127 I=1,ITOP
      IJ=L+I+1
      HHRR=HH(IJ)/R(IJ)/R(IJ)
      PROE = PIKJ(IJ-1) + PROE*HHRR
      PROC = PIKK(IJ-1) + PROC*HHRR
  127 PROD = PIK (IJ-1) + PROD*HHRR
      GOTO(131,133),IJK
  133 E(J,IDENT+12,K)=(E(J,IDENT+12,K)+PROE-PIKJ(LOOP))/DFUNCT
      E(J,IDENT+8,K)=(E(J,IDENT+8,K)+PROC-PIKK(LOOP))/DFUNCT
      E(J,IDENT+4,K)=(E(J,IDENT+4,K)+PROD-PIK(LOOP))/DFUNCT
  128 CONTINUE
  130 CONTINUE
  138 LLAST=LLAST+L
      IDENT=IDENT+1
      GOTO(20,27,36,45,139),IDENT
  139 CONTINUE
      INDATA=0
  600 INDATA=INDATA+1
  259 READ 850,KKJ,OO,WHT,ID
      IF(ID-8HEND DATA) 255,256
  255 IF(KKJ(1)-NMAX) 260,260,257
  257 PRINT 258,KKJ,OO,WHT,ID
  258 FORMAT (+N .GT. NMAX . . . LINE IGNORED+5X6I3,F12,4,F5,2,A10)
      GO TO 259
  260 M=2
      MM=4
  270 J=KKJ(MM)
      IF(J) 250,251
  251 ENG(M)=0.0
      DO 249 I=1,11
  249 Z(I,M)=0.0
      GO TO 278
  250 NL=J+KKJ(MM+MM2)+KKJ(MM+MM1)+4
      N=NL/4
```

```
      L=4*N+NL+1
      XJ=J
      XJ2=XJ*XJ+XJ
      XJ4 = XJ2*XJ2
      EJLN=E(J,L,N)
      Z(3,M)=ZETA=E(J,L+4,N)
      PZ4=E(J,L+8,N)
      Z(1,M)=XI=XJ2-ZETA
      DEL2=(ZETA*EJLN)/BP
      EN=BC*XJ2+ABC*EJLN
      IF (CAPPA) 275,275,276
  276 DEL1=(ZETA*ZETA-PZ4)/BP2-ETA*ETA
      Z(2,M)=ETA=-DEL2
      DEL3=((ETA*BP+ZETA)*ZETA-PZ4)/BP
      Z(4,M)=.0625*(XJ4-DEL1-2.*XJ2*DEL2-(1.-RR*RR)*(2.*XJ2*ZETA+2.*DEL3
     1-(1.-RR*RR)*PZ4))
      Z(5,M)=.0625*(XJ4-DEL1*2.*XJ2*DEL2-(1.-SS*SS)*(2.*XJ2*ZETA-2.*DEL3
     1-(1.-SS*SS)*PZ4))
      Z(6,M)=0.125*(XJ4+DEL1-2.*(1.-RR*SS)*XJ2*ZETA-2.*(RR-SS)*DEL3
     1*(1.-RR*RR)*(1.-SS*SS)*PZ4)
      Z(7,M)=0.25*(XJ4+DEL1-2.*XJ2*ZETA+PZ4)
      GO TO 277
  275 DEL1=(EJLN*(2.*ZETA-EJLN)-PZ4)/BP2
      Z(2,M)=ETA=DEL2
      DEL3=(EJLN*ZETA-PZ4)/BP
      Z(4,M)=.0625*(RR*RR*(XJ4-DEL1-2.*XJ2*DEL2)-(RR-2.)*(2.*RR*XJ2*ZETA
     1*2.*RR*DEL3-(RR-2.)*PZ4))
      Z(5,M)=.0625*((1.+SS)*(1.+SS)*(XJ4-2.*XJ2*ZETA+PZ4)-(1.-SS)*
     1(1.-SS)*DEL1*2.*(1.-SS*SS)*(XJ2*DEL2+DEL3))
      Z(6,M)=.125*((1.+SS)*(RR*XJ4-2.*(RR-1.)*XJ2*ZETA+(RR-2.)*PZ4)
     1*RR*((1.-SS)*DEL1-2.*SS*XJ2*DEL2)-2.*(1.+SS*(1.-RR))*DEL3)
      Z(7,M)=0.5*(XJ2*ZETA-PZ4-DEL3)
  277 Z(8,M)=XJ4*XJ2
      Z(7,M)=Z(7,M)-0.5*ZETA+0.125*XI-0.625*ETA
      Z(9,M)=XJ4*ZETA
      Z(10,M)=XJ2*PZ4
      Z(11,M)=E(J,L+12,N)
      DO 279 I=4,11
  279 EN=EN+Z(I,M)*OLDCNST(I+1)
      ENG(M)=EN
  278 MM=M=M-1
      IF(MM-1) 330,270
  330 CALC(INDATA)=CC=ENG(1)-ENG(2)
      OBS(INDATA)=OO
      NDENT(INDATA)=ID
      DIFF=OO-CC
      ADIFF=ABSF(DIFF)
      DO 331 I=1,11
  331 CONST(I,INDATA)=Z(I,1)-Z(I,2)
      CONST(12,INDATA)=0.5*(Z(1,1)-Z(1,2)+Z(2,1)-Z(2,2))
      CONST(13,INDATA)=0.5*(Z(1,1)-Z(1,2)-Z(2,1)+Z(2,2))
      IF(WHT) 203,200
  203 IF(10.0-WHT) 200,202,202
  202 IF(ADIFF*WHT-CDEVMAX) 200,201,201
```

```
201 PRINT 1000,INDATA,KKJ,OO,CC,WHT
    WHT=0.0
200 WT(INDATA)=WHT
    ENCODE (8,261,JK(1,INDATA)) KKJ(1),KKJ(2),KKJ(3)
    ENCODE (8,261,JK(2,INDATA)) KKJ(4),KKJ(5),KKJ(6)
261 FORMAT (I2,X,I2,X,I2)
    GOTO600
256 CONTINUE
    INDATA=INDATA-1
    EFIN=EPOUT = 1.0E-10
172 READ156,NK,TOL,INFO,NDELMAX,XDEVMAX,IH(10)
    IF(.NOT. TOL) TOL=0.0001
    IF(IH(10)=8HLAST FIT)173,2
174 READ151,IH
    PRINT151,IH
173 IF(IH(10)=8HEND READ)174,175
175 NOVAR = 1
    DO157I=1,13
    NVARY(I)=0
    IF(NK(I))158,157
158 N1(NOVAR)=I1(I)
    NVARY(NOVAR)=I
    NOVAR=NOVAR+1
157 CONTINUE
    SDEVMAX=XDEVMAX**2
    NOVMI = NOVAR - 1
    NOVPL=NOVMI+2
    NDEL=0
    XDATA=SUMWHT=0.0
495 NOIN=K=NOENT=NOMIN=NOMAX=0
    VAR=FLEVEL=0.0
    DO 176 I = 1,NOVPL
    DO 176 J = 1,NOVPL
176 VECTOR(I,J) = 0.0
    IF(NDEL)501,500
500 DO525N=1,INDATA
    IF(WT(N))252,253
253 NUSE(N)=0
    GO TO 254
252 NUSE(N)=1
    XDATA=XDATA+1.0
    SUMWHT=SUMWHT+WT(N)
254 NUM=0
    DO 512 I=1,NOVMI
512 DATA(I,N)=CONST(NVARY(I),N)
525 DATA(NOVAR,N)=OBS(N)=CALC(N)
501 AVEWHT=SUMWHT/ XDATA
    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 = I,NOVAR
540 VECTOR(I,J)=VECTOR(I,J)+DATA(I,N)*DATA(J,N)*WHT
```

```
 510 CONTINUE
     VECTOR(NOVPL,NOVPL) =  XDATA
     IF(INFO)580,650
 580 PRINT15,(I,I=1,NOVMI)
     PRINT 17,VECTOR(NOVAR,NOVPL),(VECTOR(I,NOVPL),I=1,NOVMI)
     NGO=0
     NOMIN=1
     NOMAX=NOVMI
     IF(NO MAX-6) 599,599,601
 601 NOMAX=6
     NGO=1
 599 PRINT 152,(I,I=NOMIN,NOMAX)
     DO 180 J=NOMIN,NOVMI
     JJ=J
     IF(JJ .GT. 6 .AND. NGO) JJ=6
 180 PRINT 153,J,(VECTOR(I,J),I=NO MIN,JJ)
     PRINT 154,(VECTOR(I,NOVAR),I=NOMIN,NOMAX)
     IF(NGO) 602,603
 602 NOMIN=7
     NOMAX=NOVMI
     NGO=0
     GO TO 599
 603 CONTINUE
     PRINT155, VECTOR(NOVAR,NOVAR)
 650 NOSTEP = -1
     NUMBER=0
     DEFR   = VECTOR(NOVPL,NOVPL) - 1.0
     DO 800  I = 1,NOVAR
     IF(VECTOR(I,I)) 792,794,810
 792 PRINT  793, I
     GOTO172
 794 PRINT 795, I
     SIGMA(I) = 1.0
     GO TO 800
 810 SIGMA(I) = SQRTF (VECTOR (I,I))
 800 VECTOR(I,I) = 1.0
     DO 830 I = 1,NOVMI
     IP1 = I + 1
     DO 830 J = IP1, NOVAR
 830 VECTOR(J,I)=VECTOR(I,J)=VECTOR(I,J) /( SIGMA(I)* SIGMA(J))
     IF(INFO)870,1001
 870 PRINT159,(I,I=1,NOVMI)
     DO 885 I=2,NOVMI
     IM1=I-1
 885 PRINT160,I,(VECTOR(I,J),J=1,IM1)
     PRINT161,(VECTOR(I,NOVAR),I=1,NOVMI)
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) * SQRTF (VECTOR(NOVAR,NOVAR)/ DEER)
     DEFR =DEFR-1.0
     IF (DEFR )  1017,1017, 1020
```

```
1017 PRINT  1019 ,NOSTEP
     GO TO 1381
1020 VMIN=VMAX=0
     NOIN=0
     DO 1050 I = 1,NOVMI
     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
     COEN(NOIN)  = VECTOR(I,NOVAR) * SIGMA(NOVAR) / SIGMA (I)
     SIGMCO(NOIN) = SQRTF(VECTOR(I,I))*SIGY/SIGMA(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 IX=8HENTERING
     IF(NOENT .LE. 0) IX=8HREMOVED
     IF(NUMBER) FLEVEL=FL
     PRINT 169,NOSTEP,IX,K,K,FLEVEL,SIGY
     DO1301J=1,NOIN
     N=INDEX(J)
1301 PRINT163,N,N1(N),COEN(J),SIGMCO(J),VECTOR(J)
     IF(NUMBER) GO TO 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) 1370,1361,1380
1361 IF (EFIN) 1380,1380,1370
1370 K = NOMAX
     NOENT = K
1391 IF(K) 1392,1392,1400
1392 PRINT 1395, NOSTEP
     GOTO172
```

```
1400 VECTOR(K,K)=VK=1.0/VECTOR(K,K)
     DO 1410   I = 1,NOVAR
     IF (I-K) 1430,1410
1430 DO 1440   J = 1, NOVAR
     IF(J.NE.K) VECTOR(I,J)=VECTOR(I,J)-VECTOR(I,K)*VECTOR(K,J)*VK
1440 CONTINUE
1410 CONTINUE
     DO 1480  I = 1, NOVAR
     IF(I.NE.K) VECTOR (I,K)  =  -  VECTOR (I,K)*VK
1480 CONTINUE
     DO 1520 J = 1, NOVAR
     IF(J.NE.K) VECTOR(K,J) =   VECTOR (K,J)*VK
1520 CONTINUE
     GOTO1001
1380 PRINT167,I5(1),I5(2),I3(NS),I5(3),XDATA,NOVMI,AVEWHT,NDELMAX,
    1XDEVMAX,STDY,NOSTEP
1381 NUMBER=1
     GO TO 1310
1580 NOT=NUM=0
     DO9200I=1,13
     CORR(I)=0.0
     IF(NK(I)) 9201,9200
9201 NUM=NUM+1
     DO 9202 J=1,NOIN
     IF(INDEX(J)-NUM) 9202,9203
9203 CORR(I)=COEN(J)
     GO TO 9200
9202 CONTINUE
     NOT=NOT + 1
     NOTIN(NOT)=NUM
9200 CONTINUE
     IF(NOT) 9211,9212
9211 DO 9210 I=1,NOT
     J=NOTIN(I)
9210 PRINT 123,J,N1(J),VECTOR(J)
9212 ADD(L1)=CORR(3)
     ADD(L2)=CORR*CORR(2)+CORR(12)
     ADD(L3)=CORR*CORR(2)+CORR(13)
9206 DO9207I=5,12
9207 ADD(I)=CORR(I-1)
     DO9208I=1,12
9208 CNST(I)=ADD(I)+OLDCNST(I)
     CNST(4)=(2.*CNST(2)*CNST-CNST(3))/(CNST-CNST(3))
     ADD(4)=CNST(4)-OLDCNST(4)
     PRINT171,(I2(I),OLDCNST(I),ADD(I),CNST(I),I=1,12)
     NFIT=50
     VFIT=DEVMAX=SWT=XIR=0.0
     DO1660N=1,INDATA
     IF(NFIT-50) 1662,1663,1663
1663 PRINT 166
     NFIT=0
1662 NFIT=NFIT+1
     WTN=NUSE(N)*WT(N)
     WHT=WTN/AVEWHT
```

```
      YPRED = 0.0
      DO 1630  I = 1,NCIN
1630  YPRED=YPRED+COEN(I)*DATA(INDEX(I),N)
      CC=CALC(N)
      OO=OBS(N)
      DIFF=OO-CC
      DEV=DIFF-YPRED
      ADEV=DEV*DEV*WTN
      IF(ADEV-DEVMAX) 1661,1610,1610
1610  NMAX=N
      DEVMAX=ADEV
1661  FPRD=OO-DEV
      IF(10.-WT(N))1652,1652,1651
1651  VFIT=VFIT+WTN*DEV**2
      XIR=XIR+1.0
      SWT=SWT+WT N
      PRINT165,N,(JK(I,N),I=1,2),WTN,OO,CC,FPRD,DIFF,YPRED,DEV,NDENT(N)
      GO TO 1660
1652  PRINT265,N,(JK(I,N),I=1,2),WTN,OO,CC,FPRD,DIFF,YPRED,DEV,NDENT(N)
1660  CONTINUE
      VFIT=VFIT*XIR/((XIR-NOIN)*SWT)
      STDFIT=SQRTF(VFIT)
      PRINT150, VFIT, STDFIT
      IF(NDELMAX-NDEL)172,172,1624
1624  IF(DEVMAX-SDEVMAX)172,172,1620
1620  NUSE(NMAX)=0
      NDEL=NDEL+1
      XDATA=XDATA-1.0
      SUMWHT=SUMWHT-WT(NMAX)
      PRINT 1000,NMAX
      GOTO495
   15 FORMAT (*1SUM OF VAR*/*0       Y*11I11)
   17 FORMAT (12F11.4)
  123 FORMAT (I11,A9* NO CORRECTION FOUND*F26,5)
  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*/I21,5I22)
  153 FORMAT (XI2,6F22,4)
  154 FORMAT (*  Y*6F20.4)
  155 FORMAT (*  Y VS Y*F15.4)
  156 FORMAT (13I1,7X,F10,18XI2,10XI5,F5,2XA8)
  159 FORMAT (*-PARTIAL CORR, COEFF.*/*0*16I8)
  160 FORMAT (I3,16F8.4)
  161 FORMAT (*  Y*16F8.4)
  163 FORMAT (I11,A9,2F17.12,F12,5)
  165 FORMAT (I5,A13,A11,   F7.2,6F10.4,A12)
  166 FORMAT(*1  RUN       UPPER       LOWER      WHT      OBS        CALC
     1    PRED       O-C         P-C         O-P*/7X2(*     N K= K=*)/)
  167 FORMAT(*1*3A8* STATE COMBINATION DIFFERENCES FOR *A8,10X*FIT*F4* D
     1ATA POINTS TO*I2* VARIABLES*9X*VERSION 6/27/67*/*     WHT NORMALIZA
     2TION*E9,2,48X*DELETES UP TO*I2* POINTS IF (O-P) GT*F6,3/ *     STD
     3DEV OF (O-C)*E10,2/*     COMPLETED*I2* STEPS*)
  169 FORMAT(*0STEP NO*I3,5X*VAR, *A8,I3/*   F LEVEL OF X=*I2,E10.2,5X
```

```
     1*STD DEV (O-P)*F9.6/10X*VARIABLE*5X*COEFFICIENT*8X*STD ERROR    DI
     2AG ELEMENT*)
  171 FORMAT(*2RESULTS*10X*COEFFICIENT*7X *OLD VALUE         CORRECTION
     1      NEW VALUE*/12(/21XA6,4X3F17.12))
  265 FORMAT (I5,A13,A11,   F9.6F10.6,A10)
  701 FORMAT (4F15)
  702 FORMAT (*ABOVE NON-EIGENVALUE NOT DIAG. AFTER 10 CYCLES*)
  795 FORMAT (* ERROR RESID SQ VAR*I3* IS NEG*)
  799 FORMAT (*0VAR*I2* IS CONST*)
  850 FORMAT (X6I3,F20.F10.2SXA8)
  904 FORMAT (*0ERROR, VMIN POS*)
  907 FORMAT (*0ERROR MOIN NEG*)
 1000 FORMAT (* LINE NO*I4* DELETED*5X6I3,2F10.4,F5.2)
 1004 FORMAT (*0Y SQUARE NEG STEP*I5)
 1019 FORMAT (*0ZERO DEG FREEDOM STEP*I3)
 1044 FORMAT (*SQUARE X-*I2* NEGATIVE STEP*I3)
 1395 FORMAT (*K=0 STEP*I3)
 9000 FORMAT (2I5,F10,3A8)
      END
```

## E. SPECFIT

The program is similar to CDFIT except that it fits frequencies to get corrections to the band origin and the rotational and centrifugal distortion constants for the upper and lower vibrational levels involved.

### STRUCTURE OF DATA DECK

| Card Type | Format | Columns | Information |
|---|---|---|---|
| 1 | I5 | 1-5 | Maximum N value of data (<48). |
| | F10 | 6-15 | If observed minus calculated is larger than this, data point is deleted on input. |
| | A5 | 16-20 | Molecule [e.g., "14NO2"]. |
| | A8 | 21-28 | Band [e.g., "(2,0,1)"]. |
| Trial constants | | | |
| 2 | 3F15 | 1-45 | Ground state A, B, C. |
| 3 | 4F15 | 1-60 | Ground state $\tau_1$, $\tau_2$, $\tau_3$, $\tau_4$. |
| 4 | 4F15 | 1-60 | Ground state $H_N$, $H_{NK}$, $H_{KN}$, $H_N$. |
| 5 | 4F15 | 1-60 | Upper state A, B, C; band origin. |
| 6 | 4F15 | 1-60 | Upper state $\tau_1$, $\tau_2$, $\tau_3$, $\tau_4$. |
| 7 | 4F15 | 1-60 | Upper state $H_N$, $H_{NK}$, $H_{KN}$, $H_K$. |
| Data (one for each data point; no more than 800 allowed) | | | |
| 8 | 6I3 | 2-19 | Values of N, $K_{-1}$, $K_{+1}$ in upper and ground vibrational states, respectively. |
| | F20 | 20-39 | Observed frequency. |
| | F10 | 40-49 | Weight assigned to this observation. |
| 9 | A8 | 73-80 | "END DATA" signals end of data. |

| Card Type | Format | Columns | Information |
|---|---|---|---|
| Parameter cards (one for each set of constants varied) | | | |
| 10 | I1 | 1 | Non-zero will enter band origin. |
| | 13I1 | 2-14 | Non-zero numbers in any of these columns will enter the corresponding upper state constants in this fit. The 13 constants are (B+C)/2, (B-C)/2, A, B, C, $\tau_1$, $\tau_2$, $\tau_3$, $\tau_4$, $H_N$, $H_{NK}$, $H_{KN}$, and $H_K$, respectively. |
| | 13I1 | 15-27 | Same as columns 2-14 except will enter corresponding ground state constants. |
| | 8I1 | 28-35 | Non-zero numbers will enter average value of upper and lower state centrifugal distortion constants, i.e., $(\tau_1'+\tau_1")/2$, $(\tau_2'+\tau_2")/2$, $(\tau_3'+\tau_3")/2$, $(\tau_4'+\tau_4")/2$, $(H_N'+H_N")/2$, $(H_{NK}'+H_{NK}")/2$, $(H_{KN}'+H_{KN}")/2$, and $(H_K'+H_K")/2$. |
| | 8I1 | 36-43 | Same as columns 28-35 except will enter half of the difference of upper and lower constants, i.e., $(\tau_1'-\tau_1")/2$, etc. |
| | I2 | 49-50 | A non-zero number will cause all of the least squares steps to be printed out. |
| | F10 | 51-60 | Tolerance for diagonal element as in CDFIT. |
| | I5 | 61-65 | Maximum number of data points to be deleted after initial fit. |
| | F5 | 66-70 | Tolerance for deleting data points. |
| | A8 | 73-80 | "END HEAD" as in CDFIT. |
| 11 | A8 | 73-80 | "LAST FIT" signals end of execution. |

## F. SPINFIT

This program fits observed spin-doublets using Eq. (27) and Eq. (29) to determine either $\varepsilon$ or $\varepsilon/A$ for each vibrational level desired. There is currently no provision for deleting data points which fit poorly. The program can also be used to predict spin-splittings on the basis of either input values of the $\varepsilon$'s or using the $\varepsilon$'s found by a fit of just one of the isotopes.

### STRUCTURE OF DATA DECK

| Card Type | Format | Columns | Information |
|---|---|---|---|
| 1 | 9A8 | 1-72 | Heading information to be printed out. |
| | A8 | 73-80 | "END HEAD" if this is last heading card. If not, program will read and print succeeding cards until "END HEAD" is encountered in columns 73-80. Columns 1-72 of the last heading card are printed at the start of each fit. |
| Data cards (one data point per card up to 99 data points allowed) | | | |
| 2 | R1 | 3 | P, Q, or R, giving $\Delta N$ for this data point. |
| | I3 | 4-6 | Value of $K_{-1}$. |
| | I3 | 7-9 | Value of ground state N. |
| | F10 | 10-19 | Observed splitting (>0 for P lines and <0 for R lines). |
| | F10 | 20-29 | Assigned weight. |
| | I2 | 41-42 | Isotope, i.e., "14" or "15." |
| 3 | A8 | 73-80 | "END DATA" signals end of data. |

| Card Type | Format | Columns | Information |
|---|---|---|---|
| Parameter cards (there can be any number, but they should be all of the same type, i.e., either 4a or 4b) | | | |
| 4a | For fitting data from only one isotope to determine $\varepsilon'$ and/or $\varepsilon''$ and/or for predicting spin-doubling for one isotope. | | |
| | 4I1 | 1-4 | A non-zero number will enter the corresponding variable in this fit. The four possible variables are $\varepsilon''$, $\varepsilon'$, $(\varepsilon'+\varepsilon'')/2$, and $(\varepsilon'-\varepsilon'')/2$. If all four columns are left blank, the program will predict spin-splittings using the values of $\varepsilon$ given in columns 11-30. |
| | I6 | 5-10 | Maximum value of K for which spin-splittings will be predicted starting with K = 1. If left blank, will not predict any splittings. |
| | 2F10 | 11-30 | Initial values of $\varepsilon''$ and $\varepsilon'$ for this fit. |
| 4b | For fitting both isotopes to determine $^{14}\varepsilon''/^{14}A'' = {}^{15}\varepsilon''/^{15}A''$ and/or $^{14}\varepsilon'/^{14}A' = {}^{15}\varepsilon'/^{15}A'$. | | |
| | 4I1 | 1-4 | Same as for card type 4a except that the four possible variables are $\varepsilon''/A''$, $\varepsilon'/A'$, $(\varepsilon'/A'+\varepsilon''/A'')/2$, and $(\varepsilon'/A'-\varepsilon''/A'')/2$. |
| | | 5-10 | Blank. |
| | 2F10 | 11-30 | Initial values of $\varepsilon''/A''$ and $\varepsilon'/A'$ for this fit. |
| | 4F10 | 31-70 | Values of $^{14}A''$, $^{14}A'$, $^{15}A''$, $^{15}A'$. |
| 5 | A8 | 73-80 | "LAST FIT" signals last fit has been performed on this set of data. |
| 6 | Start new set of data with another card type 1, or blank card to stop execution. | | |

## G. PLOTZ

For each specified field strength this program calculates the transition probabilities for the Zeeman components of specified transitions and plots a predicted spectrum, integrating over a Gaussian, Lorentzian, or triangular slit function to determine the apparent percentage absorption at each point. It also can plot a vertical line at the center of each component which is proportional to the absorption by that component.

STRUCTURE OF DATA DECK

| Card Type | Format | Columns | Information |
|---|---|---|---|
| 1 | 2F10 | 1-20 | Values of $\varepsilon$" and $\varepsilon$' to be used for the following data. |
| | 2A8 | 23-38 | Identification [e.g., "(2,0,1) OF 14NO2"]. |
| | R1 | 41 | Slit function to be used: "G" for Gaussian, "L" for Lorentzian, or "T" for triangular. |
| | R1 | 44 | If left blank, program will plot a vertical line at the center of each component. The height of each line is proportional to the percentage absorption by that component. The envelope of the resulting predicted spectrum is then plotted. An "F" suppresses plotting of the vertical lines; an "E" suppresses plotting of the envelope. |
| | F5 | 45-50 | Wavenumber scale giving number of inches on the plot for each $cm^{-1}$. (The total width of the plot must be less than 27 inches.) |
| | F5 | 51-55 | Intensity scale giving number of inches for height of a 100% absorbing line. |

| Card Type | Format | Columns | Information |
|---|---|---|---|
| | F5 | 56-60 | Half-width at half-intensity of slit function. |
| | F5 | 61-65 | Value of $\alpha$ [cf. Eq. (66)]. |
| | I5 | 66-70 | Non-zero number to suppress printing of positions and transition probabilities of individual Zeeman components. |
| | F5 | 71-75 | Value of ground state A for spectrum to be plotted. |
| | F5 | 76-80 | Value of (B+C)/2 in the ground state for spectrum to be plotted. |
| 2 | 6F10 | 1-60 | Up to six magnetic fields at which the Zeeman spectrum is to be calculated and plotted. Only the first field may be zero. |

Data cards (one for each asymmetric rotor transition which is to be included in the spectra; as many as desired)

| | | | |
|---|---|---|---|
| 3 | R1 | 4 | "P", "Q", or "R", signifying $\Delta N = -1$, 0, or +1. |
| | I3 | 5-7 | Value of $K_{-1}$. |
| | I3 | 8-10 | Value of N in ground state. |
| | F10 | 11-20 | Predicted asymmetric top frequency. |

4 Blank card to signal end of data.

5 Data for next set of plots, starting with new card type 1, or blank card to stop execution.

A listing of the program PLOTZ follows.

```
      PROGRAM PLOTZ
      COMMON DELNU(6),XKAP(2),XNU(2),XN,XN1,XM,XM1,SPIN1,SPIN2,PQR,
     2FRACT,NDELN,NLINES,DELM,JMAX,KK,NOPRINT
      DIMENSION FIELD (6),IHEAD(2),EPS(2)
      COMMON/4/FRQ(6,250),ZINT(6,250),FNU(1500),A(1500),MM(6),J,LABEL(2)
     1,XTEST,YTEST
      EQUIVALENCE (FRQ,FNU),(ZINT,A)
      COMMON/1/XX(6,1500),YY(6,1500)
      COMMON/2/SY,SX,SYI,SXI,SC25,YC,YS,METHOD,SCALE,HS,GAM,ISPRS
      COMMON/5/DUMMY(1),SHAPE(500),NPTS,FGAM,XGAM,ALPHA,IFLIN,IFENV
      CALL PLOT( 0.,31.,0,100.,.100,)
      CALL PLOT(0.,0.,1)
      CALL PLOT(4.,2.,2)
      STATWT=1,43883/300,
      MM(1)=NPLOTS=0
    1 READ 9000,EPS,IHEAD,METHOD,ISPRS,SCALE,HS,GAM,ALPHA,NOPRINT
     1,AZERO,BBAR
9000 FORMAT (2F10.2X2A8,2XR1,2XR1,X4F5,I5,2F5)
      IF(EPS) 4,5
    5 CALL PLOT (15.,0.,-1)
      PRINT 9005
9005 FORMAT (*5*)
      STOP
    4 NPLOTS=NPLOTS+1
      NUB=50*NPLOTS
      CALL PLOT(NUB,0.,3)
      IF( .NOT. AZERO) AZERO=8.002509
      IF( .NOT. BBAR ) BBAR =0.4220786
      READ 9003, FIELD
9003 FORMAT (8F10)
      DELNU(1)=0.0000467536*FIELD(1)
      DO 20 I=2,6
      MM(I)=0
      DELNU(I)=0.0000467536*FIELD(I)
      IF(DELNU(I)) 20,21
   20 CONTINUE
      I=7
   21 JMAX=I-1
      IFLIN=ISPRS=22
      IFENV=IFLIN+1
      SC25=0.25/SCALE
      SX=100.*SCALE
      SY=100.*HS
      SXI=1.0/SX
      SYI=1.0/SY
      SYI5=SYI*5.0
      YC=-25.*SYI
      YS=- 5.*SYI
      XTEST=SXI
      YTEST=0.01
      FGAM=IGAM=2.0*GAM*SX*0.5
      XGAM=FGAM*SXI*0.5
      FGAM=0.5/XGAM
      CALL PROFILE
```

```
      IF(NOPRINT) PRINT 9006,IHEAD,(FIELD(J),J=1,JMAX)
 9006 FORMAT(*4ZEEMAN COMPONENTS WILL BE CALCULATED AND PLOTTED FOR THE
     1FOLLOWING LINES OF THE *2A8/*0CUMULATIVE NO, OF COMPONENTS AT THE
     2FOLLOWING FIELDS*6F6/)
    2 READ 9001,NDEL,KK,NN,FREQ
 9001 FORMAT(3XR1,2I3,F10)
      NDELN=NDEL-1RQ
      IF(NDELN/2) GO TO 6
      FKJ=BBAR*(NN*NN*NN)*(AZERO-BBAR)*(KK**2)
      BOLTZ=EXPF(-STATWT*FKJ)
      NLINES=0
      FF=INTF(FREQ)
      FRACT=FREQ-FF
      XK2=KK**2
      XN=NN
      XN2=XN**2
      XN1=NN*NDELN
      XN12=XN1*XN1
      XKAP(1)=0,5*EPS(1)*XK2/(XN2*XN)
      XKAP(2)=0,5*EPS(2)*XK2/(XN12*XN1)
      XNU(1)=     XKAP(1)*(XN-0,5)
      XNU(2)=     XKAP(2)*(XN1-0,5)
      IF(NOPRINT) 24,25
   24 PRINT 9008,NDEL,KK,NN,FREQ
 9008 FORMAT (5XR1,I1,*(*I2*)*F15,4)
      GO TO 26
   25 PRINT 9002,NDEL,KK,NN,IHEAD,FREQ,(FIELD(I),I=1,JMAX)
 9002 FORMAT(*5*/*0ZEEMAN FREQUENCIES AND INTENSITIES FOR *R1,I1*(*I2*)
     2OF *2A8*  LINE CENTER =*F10,4/*9*10X*MN* MN**F10,8F13)
   26 GO TO (100,200,300),(NDELN-2)
  100 PQR=0,50*(XN2-XK2)/(4,0*XN2**2-XN2)
      MMIN1=-NN
      MMIN2=MMAX2=MMIN3=MMIN1+1
      MMAX1=NN-2
      MMAX3=MMAX1+1
      GO TO 400
  200 PQR=0,50*XK2/(XN2*XN)**2
      MMIN3=MMIN1=MMIN2=-NN
      MMAX2=MMAX3=NN
      MMAX1=MMAX2-1
      GO TO 400
  300 PQR=(XN12-XK2)/(8,*XN12*(XN2*XN+XN-0,75))
      MMIN3=MMAX3=MMIN1=MMIN2=-NN
      MMAX1=MMAX2=NN
      GO TO 400
  400 CONTINUE
      SPIN1=-1,0
      DO 401 K=1,2
      SPIN1=SPIN2=-SPIN1
      DELM=-1,0
      DO 401 I=1,2
      DELM=-DELM
      DO 401 M=MMIN1,MMAX1
      XM=DELM*M
```

```
      XM1=XM+DELM
  401 CALL ZEEMAN
      IF(.NOT. KK) GO TO 404
      SPIN1=+1.0
      SPIN2=-1.0
      DO 402 M=MMIN2,MMAX2
      XM=XM1=M
  402 CALL ZEEMAN
      SPIN1=-1.0
      SPIN2=+1.0
      DO 405 M=MMIN3,MMAX3
      XM=XM1=M
  405 CALL ZEEMAN
  404 CONTINUE
      DO 403 J=1,JMAX
      DO 406 I=1,NLINES
      IP1=I+1
      DO 406 K=IP1,NLINES
      SUMA=ZINT(J,K)+ZINT(J,I)+1.0E-10
      DIFF=FRQ(J,K)-FRQ(J,I)
      GO TO (407,409,409,406),(DIFF/XTEST+3.0)
  407 FRQ(J,I)=FRQ(J,K)
      FRQ(J,K)=FRQ(J,K)-DIFF
      DIFF=-DIFF
      ZINT(J,I)=ZINT(J,K)
      ZINT(J,K)=SUMA-ZINT(J,K)
      GO TO 406
  409 FRQ(J,I)=(FRQ(J,I)+ZINT(J,I)+FRQ(J,K)+ZINT(J,K))/SUMA
      ZINT(J,I)=SUMA
      ZINT(J,K)=0.0
  406 CONTINUE
      DO 408 I=1,NLINES
      IF(ZINT(J,I) .LT. YTEST) GO TO 408
      N=MM(J)=MM(J)+1
      XX(J,N)=FRQ(J,I)+FF
      YY(J,N)=ZINT(J,I)+BOLTZ
  408 CONTINUE
  403 CONTINUE
      IF(NOPRINT) 27,28
   27 PRINT 9009,(MM(J),J=1,JMAX)
 9009 FORMAT (+++52X6I6)
      GO TO 2
   28 PRINT 9007,(MM(J),J=1,JMAX)
 9007 FORMAT (+0NLINES(FIELD) =+6I13)
      GO TO 2
    6 DO 10 J=1,JMAX
      NM=MM(J)
      DO 9 I=1,NM
      FNU(I)=XX(J,I)
    9 A(I)=YY(J,I)
      ENCODE (8,9004,LABEL(1)) FIELD(J)
 9004 FORMAT (+H =+F5)
      LABEL(2)=8H GAUSS
   10 CALL SUM
```

```
      GO TO 1
      END
      SUBROUTINE ZEEMAN
      COMMON DELNU(6),XKAP(2),XNU(2),XN(2),XM(2),S(2),PQR,FRACT,NDEL
     1,NLINES,DELM,JMAX,KK,NOPRINT
      COMMON/4/FRQ(6,250),ZINT(6,250),DUM(11)
      DIMENSION V1(2),V2(2),V3(2),EP(2),EM(2),E(2)
      NLINES=NLINES+1
      DM=DELM*XM(1)
      DMP=DM+DELM
      DMM=DM-DELM
      DO 1100 J=1,JMAX
      IF(KK) 3,4
    4 IF(J .EQ. 1) GO TO 3
      DO 6 I=2,JMAX
      FRQ (I,NLINES)=FRQ (1,NLINES)
    6 ZINT(I,NLINES)=ZINT(1,NLINES)
      GO TO 7
    3 CONTINUE
      D=DELNU(J)
      DO 1101 I=1,2
      XMN=XM(I)
      E(I)=-0.50*XKAP(I)*S(I)*SQRTF(D*D+2.0*D*XKAP(I)*
     2(XMN+0.5*S(I))*      XNU(I)**2)
      IF(XN(I) .EQ. S(I)*XMN)  E(I)=S(I)*(XKAP(I)*XMN+D)
      IF(S(I) .LT. 0.0) XMN=XMN-1.0
      V1(I)=XKAP(I)*XMN  +D
      V2(I)=-V1(I)-XKAP(I)
      V3(I)=XKAP(I)*SQRTF(XN(I)**2+XN(I)-XMN*(XMN+1.0))
      EP(I)=0.5*(V1(I)+V2(I)) + SQRTF(0.25*(V1(I)-V2(I))**2+V3(I)**2)
      IF( .NOT. V3(I) ) EP(I) = V1(I)
1101  EM(I)=-EP(I)-V1(I)-V2(I)
      FRQ(J,NLINES)=FRACT*E(2)-E(1)
      IF(S(1)*S(2)) 2000,1,1000
    1 IF(S(1))4000,2,3000
1000  CONTINUE
      R1=V3(1)/(V2(1)-EP(1))
      R12=R1**2
      R2=V3(2)/(V2(2)-EP(2))
      R22=R2**2
      C1=1.0/((1.0+R12)*(1.0+R22))
      C2=C1*R12*R22
      C3=2.0*R1*R2*C1
      IF(NDEL) 1001,1002,1003
1001  D1=(XN(1)-DM)*(XN(1)-DM-1.0)
      D2=(XN(1)-DMP)*(XN(1)-DMP-1.0)
      GO TO 1100
1002  D1=(XN(1)-DM)*(XN(1)+DM+1.0)
      D2=(XN(1)-DMP)*(XN(1)+DMP+1.0)
      GO TO 1100
1003  D1=(XN(1)+DM+1.0)*(XN(1)+DM+2.0)
      D2=(XN(1)+DMP+1.0)*(XN(1)+DMP+2.0)
      GO TO 1100
2000  CONTINUE
```

```
      R1=V3(1)/(V1(1)-EM(1))
      R12=R1**2
      R2=V3(2)/(V1(2)-EM(2))
      R22=R2**2
      C2=1.0/((1.0+R12)*(1.0+R22))
      C1=C2*R12*R22
      C3=2.0+R1*R2*C2
      IF(NDEL) 2001,2002,2003
2001  D1=(XN(1)-DMM)*(XN(1)-DMM+1.0)
      D2=(XN(1)-DM)*(XN(1)-DM+1.0)
      GO TO 1100
2002  D1=(XN(1)-DMM)*(XN(1)+DMM+1.0)
      D2=(XN(1)-DM)*(XN(1)+DM+1.0)
      GO TO 1100
2003  D1=(XN(1)+DMM+1.0)*(XN(1)+DMM+2.0)
      D2=(XN(1)+DM+1.0)*(XN(1)+DM+2.0)
      GO TO 1100
3000  CONTINUE
      R1=V3(1)/(V2(1)-EP(1))
      R12=R1**2
      R2=V3(2)/(V1(2)-EM(2))
      R22=R2**2
      R3=1.0/((1.0+R12)*(1.0+R22))
      C1=R22*R3
      C2=R12*R3
      C3=2.0+R1*R2*R3
      IF(NDEL) 3001,3002,3003
3001  XNP=XN(1)+XM(1)
      D1=XNP*(XNP-1.0)
      D2=XNP*(XNP+1.0)
      GO TO 1100
3002  XNP=XN(1)+XM(1)
      XNM=XN(1)-XM(1)
      D1=XNP*(XNM+1.0)
      D2=(XNP+1.0)*XNM
      GO TO 1100
3003  XNM1=XN(1)-XM(1)+1.0
      D1=XNM1*(XNM1+1.0)
      D2=XNM1*(XNM1-1.0)
      GO TO 1100
4000  CONTINUE
      R1=V3(1)/(V1(1)-EM(1))
      R12=R1**2
      R2=V3(2)/(V2(2)-EP(2))
      R22=R2**2
      R3=1.0/((1.0+R12)*(1.0+R22))
      C1=R12*R3
      C2=R22*R3
      C3=2.0+R1*R2*R3
      IF(NDEL) 4001,4002,4003
4001  XNM=XN(1)-XM(1)
      D1=XNM*(XNM+1.0)
      D2=XNM*(XNM-1.0)
      GO TO 1100
```

```
4002 XNP=XN(1)+XM(1)
     XNM=XN(1)-XM(1)
     D1=(XNM+1.0)*XNP
     D2=XNM*(XNP+1.0)
     GO TO 1100
4003 XNP1=XN(1)+XM(1)+1.0
     D1=XNP1*(XNP1-1.0)
     D2=XNP1*(XNP1+1.0)
1100 ZINT(J,NLINES)=PQR*(C1*D1+C2*D2+C3*SQRTF(D1*D2))
   7 CONTINUE
     IF(NOPRINT) GO TO 2
     PRINT 9000,S,XM,(FRQ(J,NLINES),ZINT(J,NLINES),J=1,JMAX)
9000 FORMAT (XF2*/2--F2*/2*2F4,9(0P,F9,4,3P,F4))
   2 RETURN
     END
     SUBROUTINE SUM
     DIMENSION POS(3000)
     COMMON/4/XNU(1500),A(1500),NN(6),NOPLOT,LABEL(2),XTEST,YTEST
     COMMON/2/SY,SX,SYI,SXI,SC25,YC,YS,METHOD,SCALE,HS,GAM,ISPRS
     COMMON/3/DUMMY(1),SHAPE(500),NPTS,FGAM,XGAM,ALPHA,IFLIN,IFENV
     I=NN(NOPLOT)
     DO 4 J=1,I
     L=J+1
     DO 4 K=L,I
     SUMA=A(J)+A(K)
     XN=XNU(K)-XNU(J)
     GO TO (2,3,3,4),(XN/XTEST+3.0)
   2 XNU(J)=XNU(J)+XN
     XNU(K)=XNU(K)-XN
     XN=-XN
     A(J)=A(K)
     A(K)=SUMA-A(K)
     GO TO 4
   3 XNU(J)=(XNU(J)*A(J)+XNU(K)*A(K))/SUMA
     A(J)=SUMA
     A(K)=00.0
   4 CONTINUE
     II=0
     DO 8 J=1,I
     IF(A(J) .LT. YTEST) GO TO 8
     II=II+1
     XNU(II)=XNU(J)
     A(II)=A(J)
   8 CONTINUE
     I=II
     PRINT 202,I,LABEL,(XNU(J),A(J),J=1,I)
 202 FORMAT (*--*I4* FREQUENCIES PLOTTED AT *2A8/(8(XF10.4,F6.3)))
     CALL PLOT(0.,0.,0)
     X=0.0
     DO 33 N=1,2
     CALL CHAR(-.75,X,LABEL(N),8,0.,-1,15
  33 X=X+1.5
     CALL PLOT(0.,0.,2)
     Z=INTF(XNU(1)-0.2)
```

```
      LT=XT=INTF(XNU(I)+1.2-Z)
      LE=LT+10
      SIZE=XT*SCALE
      X=-.1
      L=0
      DO 5 K=L,LE
      X=X+.1
      Y= YS
      CALL PLOT(0.,X,1,SY,SX)
      IF(K .EQ. K/5*5) Y=Y+YS
      CALL PLOT(Y,X,1)
    5 CALL PLOT(0.,X,1)
      LF=LT+1
      NR=Z+LT
      XC=LT
      X=XC-SC25
      XC=XC+1.3*SC25
      CALL CHAR( YC,XC,2HCM,2,0.,.1,.1)
      XC=XC+SC25
      YY=0.75*YC
      CALL CHAR(YY,XC,2H-1,2,0.,.06,.06)
      DO 6 K=1,LF
      ENCODE(4,200,LA)NR
  200 FORMAT(I4)
      CALL CHAR (YC,X,LA,4,0.,.1,.1)
      NR=NR-1
    6 X=X-1.
      MAXPOS=SX
      LIM=LE*SCALE*10.
      IF(LIM .GT. 3000) LIM = 3000
      DO 7 IN=1,LIM
    7 POS(IN)=0.
      MIN=-NPTS
      CALL PLOT (0.0,0.,2)
      DO 9 K=1,I
      XX=XNU(K)-Z
      IN=XX*SX
      YY=A(K)
      Y=1.0-EXPF(-0.1*ALPHA*YY)
      IF(IFLIN) 30,9
   30 CALL PLOT (0.0,XX,1)
      CALL PLOT ( Y ,XX,1)
      CALL PLOT (0.0,XX,1)
    9 POS(IN)=POS(IN)+YY
      IF(.NOT. IFENV) GO TO 20
      DO 21 IN=1,LIM
   21 IF(POS(IN)) GO TO 22
   22 MIN=IN-1
      DO 23 IN=1,LIM
   23 IF(POS(LIM-IN)) GO TO 24
   24 MAX=LIM-IN+1
      DO 12 IN=MIN,MAX
   12 POS(IN)=1.0-EXPF(-ALPHA*POS(IN))
      MIN=MIN-NPTS
```

```
      IF(MIN .LE. NPTS) MIN=NPTS+1
      MAX=MAX+NPTS
      IF(MAX .GE. (LIM-NPTS)) MAX=LIM-NPTS-1
      X=(MIN-1)*SXI
      CALL PLOT(0.0,X ,1)
      MIN1=-NPTS
      MAX1= NPTS
      DO 10 IN=MIN,MAX
      X=X+SXI
      Y=0
      DO 11 IM=MIN1,MAX1
   11 Y=Y+POS(IN+IM)*SHAPE(XABSF(IM))
   10 CALL PLOT(Y,X,1)
   20 CALL PLOT(0.,0.,2)
      X=0.0
      Y=-4.
      IF(SIZE .GT. 12.0) GO TO 25
      MM=NOPLOT-(NOPLOT/2)*2
      Y=MM*4-4
      X= -30*MM+15
   25 CONTINUE
      CALL PLOT( Y , X,0.100.,100.)
      CALL PLOT(0.,0.,2)
      RETURN
      END
      SUBROUTINE PROFILE
      COMMON/2/SY,SX,SYI,SXI,SC25,YC,YS,METHOD,SCALE,HS,GAM,ISPRS
      COMMON/5/DUMMY(1),SHAPE(500),NPTS,FGAM,XGAM,ALPHA,IFLIN,IFENV
      GAM2=XGAM**2
      GAM2LN2=0.69315/GAM2
      N=0
      SHAPE(N)=1.0
      TEST=      SYI
      IF(METHOD-35)  2,3,4
    4 ASSIGN 400 TO NGO
      NAME=8HTRIANGLE
      GO TO 5
    3 ASSIGN 300 TO NGO
      NAME=8HLORENTZ
      GO TO 5
    2 ASSIGN 200 TO NGO
      NAME=8HGAUSSIAN
    5 CONTINUE
      X=0.0
      DO 100 I=1,500
      X=X+SXI
      X2=X**2
      GO TO NGO
  400 SHAPE(I)=1.0-X*FGAM
      GO TO 102
  300 SHAPE(I)=GAM2/(X2+GAM2)
      GO TO 102
  200 SHAPE(I)=EXP(-GAM2LN2*X2)
  102 IF(SHAPE(I)-TEST) 101,100,100
```

```
100 CONTINUE
    NPTS=500
101 NPTS=1
    PRINT 500,SCALE,HS,ALPHA,NAME,XGAM,GAM,NPTS,(SHAPE(J),J=N,NPTS)
500 FORMAT(*1THE NEXT LINES WILL BE PLOTTED AT*F6.3* CM-1/INCH AND 100
   1% ABSORBING LINES WILL BE*F5.2* INCHES HIGH*/* THE LINES ARE ASSUM
   2ED TO BE DELTA FUNCTIONS WITH HEIGHTS GIVEN BY (1.-EXPF(-*F5.3,10H
   3*<M>**2))*/5X* WHERE <M> IS THE DIPOLE MOMENT MATRIX ELEMENT*/* A*
   4A9* SLIT FUNCTION WAS USED TO INTEGRATE OVER THESE LINES,*/4X*ITS
   5HALF-WIDTH AT HALF-INTENSITY IS*F7.4* CM-1 (INPUT AS*F7.4* CM-1),*
   6/* THERE ARE A MAXIMUM OF*I4* PLOTTER UNITS FROM EACH LINE CENTER
   7 TO ITS LAST POINT PLOTTED,*/6X*THE INTENSITIES AT EACH OF THESE P
   8OINTS FOR A LINE OF UNIT HEIGHT ARE*/(10X20F6.3))
    RETURN
    END
```

## APPENDIX II

### GROUND STATE COMBINATION DIFFERENCES FOR 14NO2

| UPPER | | | LOWER | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| N | K- | K+ | N | K- | K+ | OBSERVED | OBS-CALC | WEIGHT | |
| 1 | 1 | 1 | 2 | 0 | 2 | 5,877769 | -0,000000 | 1000000 | 14 MICRO |
| 3 | 1 | 3 | 4 | 0 | 4 | 4,132328 | -0,000000 | 2000000 | 14 MICRO |
| 7 | 1 | 7 | 8 | 0 | 8 | 0,510467 | 0,000006 | 250000 | 14 MICRO |
| 10 | 0 | 10 | 9 | 1 | 9 | 1,361426 | 0,000028 | 40000 | 14 MICRO |
| 21 | 2 | 20 | 22 | 1 | 21 | 1,306371 | -0,000003 | 40000 | 14 MICRO |
| 24 | 1 | 23 | 23 | 2 | 22 | 0,887373 | -0,000003 | 40000 | 14 MICRO |
| 39 | 3 | 37 | 40 | 2 | 38 | 0,534214 | 0,000001 | 900 | 14 MICRO |
| 46 | 0 | 46 | 44 | 0 | 44 | 75,4661 | 0,0001 | 0,24 | 14NO2 GS |
| 42 | 0 | 42 | 40 | 0 | 40 | 68,9791 | 0,0204 | 0,17 | 14NO2 GS |
| 38 | 0 | 38 | 36 | 0 | 36 | 62,4419 | 0,0041 | 0,10 | 14NO2 GS |
| 34 | 0 | 34 | 32 | 0 | 32 | 55,9010 | 0,0034 | 0,82 | 14NO2 GS |
| 32 | 0 | 32 | 30 | 0 | 30 | 52,6209 | 0,0026 | 0,46 | 14NO2 GS |
| 30 | 0 | 30 | 28 | 0 | 28 | 49,3302 | -0,0016 | 0,46 | 14NO2 GS |
| 28 | 0 | 28 | 26 | 0 | 26 | 46,0366 | -0,0010 | 1,00 | 14NO2 GS |
| 26 | 0 | 26 | 24 | 0 | 24 | 42,7336 | -0,0014 | 1,00 | 14NO2 GS |
| 20 | 0 | 20 | 18 | 0 | 18 | 32,7793 | 0,0039 | 0,42 | 14NO2 GS |
| 18 | 0 | 18 | 16 | 0 | 16 | 29,4409 | 0,0022 | 1,00 | 14NO2 GS |
| 12 | 0 | 12 | 10 | 0 | 10 | 19,3873 | 0,0024 | 0,17 | 14NO2 GS |
| 6 | 0 | 6 | 4 | 0 | 4 | 9,2712 | -0,0112 | 0,82 | 14NO2 GS |
| 2 | 0 | 2 | 0 | 0 | 0 | 2,5135 | -0,0189 | 0,17 | 14NO2 GS |
| 47 | 1 | 47 | 45 | 1 | 45 | 76,8945 | -0,0073 | 0,20 | 14NO2 GS |
| 46 | 1 | 45 | 44 | 1 | 43 | 77,1156 | 0,0043 | 0,73 | 14NO2 GS |
| 45 | 1 | 45 | 43 | 1 | 43 | 73,6207 | -0,0079 | 0,31 | 14NO2 GS |
| 44 | 1 | 43 | 42 | 1 | 41 | 73,7948 | 0,0042 | 0,77 | 14NO2 GS |
| 43 | 1 | 43 | 41 | 1 | 41 | 70,3499 | -0,0021 | 0,13 | 14NO2 GS |
| 42 | 1 | 41 | 40 | 1 | 39 | 70,4552 | -0,0049 | 0,87 | 14NO2 GS |
| 40 | 1 | 39 | 38 | 1 | 37 | 67,1206 | 0,0003 | 0,33 | 14NO2 GS |
| 39 | 1 | 39 | 37 | 1 | 37 | 63,7889 | 0,0007 | 0,13 | 14NO2 GS |
| 38 | 1 | 37 | 36 | 1 | 35 | 63,7702 | -0,0014 | 0,51 | 14NO2 GS |
| 37 | 1 | 37 | 35 | 1 | 35 | 60,5071 | 0,0061 | 0,24 | 14NO2 GS |
| 36 | 1 | 35 | 34 | 1 | 33 | 60,4167 | 0,0022 | 0,67 | 14NO2 GS |
| 32 | 1 | 31 | 30 | 1 | 29 | 53,6810 | 0,0035 | 0,46 | 14NO2 GS |
| 30 | 1 | 29 | 28 | 1 | 27 | 50,3017 | 0,0029 | 1,00 | 14NO2 GS |
| 28 | 1 | 27 | 26 | 1 | 25 | 46,9138 | -0,0000 | 1,46 | 14NO2 GS |
| 25 | 1 | 25 | 23 | 1 | 23 | 40,7027 | -0,0029 | 0,18 | 14NO2 GS |
| 23 | 1 | 23 | 21 | 1 | 21 | 37,4019 | 0,0069 | 0,47 | 14NO2 GS |
| 22 | 1 | 21 | 20 | 1 | 19 | 36,7240 | -0,0034 | 0,18 | 14NO2 GS |
| 21 | 1 | 21 | 19 | 1 | 19 | 34,0835 | 0,0020 | 1,00 | 14NO2 GS |
| 19 | 1 | 19 | 17 | 1 | 17 | 30,7670 | 0,0018 | 0,67 | 14NO2 GS |
| 18 | 1 | 17 | 16 | 1 | 15 | 29,9089 | -0,0061 | 0,67 | 14NO2 GS |
| 16 | 1 | 15 | 14 | 1 | 13 | 26,5007 | -0,0031 | 1,00 | 14NO2 GS |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 15 | 1 | 15 | 13 | 1 | 13 | 24,1250 | -0,0001 | 1,00 | 14NO2 GS |
| 13 | 1 | 13 | 11 | 1 | 11 | 20,7952 | -0,0066 | 0,46 | 14NO2 GS |
| 12 | 1 | 11 | 10 | 1 | 9 | 19,6712 | -0,0020 | 0,18 | 14NO2 GS |
| 11 | 1 | 11 | 9 | 1 | 9 | 17,4757 | -0,0009 | 0,99 | 14NO2 GS |
| 9 | 1 | 9 | 7 | 1 | 7 | 14,1500 | 0,0002 | 1,00 | 14NO2 GS |
| 7 | 1 | 7 | 5 | 1 | 5 | 10,8203 | -0,0014 | 0,82 | 14NO2 GS |
| 5 | 1 | 5 | 3 | 1 | 3 | 7,4898 | -0,0028 | 0,18 | 14NO2 GS |
| 4 | 1 | 3 | 2 | 1 | 1 | 5,9854 | -0,0051 | 0,82 | 14NO2 GS |
| 3 | 1 | 3 | 1 | 1 | 1 | 4,1758 | 0,0130 | 0,18 | 14NO2 GS |
| 7 | 1 | 7 | 6 | 1 | 5 | 5,3330 | -0,0057 | 0,17 | 14NO2 GS |
| 6 | 1 | 5 | 5 | 1 | 5 | 5,4873 | 0,0043 | 0,18 | 14NO2 GS |
| 5 | 1 | 5 | 4 | 1 | 3 | 3,9387 | 0,0087 | 0,18 | 14NO2 GS |
| 4 | 1 | 3 | 3 | 1 | 3 | 3,5632 | 0,0006 | 0,58 | 14NO2 GS |
| 3 | 1 | 3 | 2 | 1 | 1 | 2,4253 | -0,0026 | 0,85 | 14NO2 GS |
| 2 | 1 | 1 | 1 | 1 | 1 | 1,7390 | 0,0041 | 1,13 | 14NO2 GS |
| 48 | 2 | 46 | 46 | 2 | 44 | 80,8618 | -0,0049 | 0,42 | 14NO2 GS |
| 47 | 2 | 46 | 45 | 2 | 44 | 77,9974 | -0,0014 | 0,41 | 14NO2 GS |
| 46 | 2 | 44 | 44 | 2 | 42 | 77,4641 | 0,0014 | 0,17 | 14NO2 GS |
| 45 | 2 | 44 | 43 | 2 | 42 | 74,6917 | 0,0073 | 0,17 | 14NO2 GS |
| 44 | 2 | 42 | 42 | 2 | 40 | 74,0491 | -0,0034 | 1,28 | 14NO2 GS |
| 43 | 2 | 42 | 41 | 2 | 40 | 71,3944 | 0,0294 | 0,24 | 14NO2 GS |
| 42 | 2 | 40 | 40 | 2 | 38 | 70,6298 | -0,0072 | 0,17 | 14NO2 GS |
| 38 | 2 | 36 | 36 | 2 | 34 | 63,7914 | -0,0027 | 0,33 | 14NO2 GS |
| 33 | 2 | 32 | 31 | 2 | 30 | 54,7041 | 0,0053 | 1,00 | 14NO2 GS |
| 32 | 2 | 30 | 30 | 2 | 28 | 53,5220 | 0,0055 | 0,60 | 14NO2 GS |
| 30 | 2 | 28 | 28 | 2 | 26 | 50,0893 | -0,0025 | 0,13 | 14NO2 GS |
| 28 | 2 | 26 | 26 | 2 | 24 | 46,6690 | -0,0005 | 1,37 | 14NO2 GS |
| 26 | 2 | 24 | 24 | 2 | 22 | 43,2496 | -0,0009 | 1,00 | 14NO2 GS |
| 25 | 2 | 24 | 23 | 2 | 22 | 41,2985 | 0,0050 | 1,00 | 14NO2 GS |
| 19 | 2 | 18 | 17 | 2 | 16 | 31,2068 | 0,0005 | 0,82 | 14NO2 GS |
| 18 | 2 | 16 | 16 | 2 | 14 | 29,6213 | 0,0041 | 0,82 | 14NO2 GS |
| 15 | 2 | 14 | 13 | 2 | 12 | 24,4665 | -0,0028 | 0,33 | 14NO2 GS |
| 14 | 2 | 12 | 12 | 2 | 10 | 22,8281 | 0,0006 | 0,77 | 14NO2 GS |
| 12 | 2 | 10 | 10 | 2 | 8 | 19,4372 | -0,0014 | 1,00 | 14NO2 GS |
| 11 | 2 | 10 | 9 | 2 | 8 | 17,7300 | 0,0052 | 0,82 | 14NO2 GS |
| 10 | 2 | 8 | 8 | 2 | 6 | 16,0555 | 0,0024 | 0,42 | 14NO2 GS |
| 9 | 2 | 8 | 7 | 2 | 6 | 14,3494 | -0,0010 | 0,29 | 14NO2 GS |
| 8 | 2 | 6 | 6 | 2 | 4 | 12,6724 | 0,0021 | 0,17 | 14NO2 GS |
| 4 | 2 | 2 | 2 | 2 | 0 | 5,9095 | -0,0014 | 0,70 | 14NO2 GS |
| 11 | 2 | 10 | 10 | 2 | 8 | 9,2599 | 0,0023 | 0,17 | 14NO2 GS |
| 10 | 2 | 8 | 9 | 2 | 8 | 8,4750 | 0,0077 | 0,17 | 14NO2 GS |
| 9 | 2 | 8 | 8 | 2 | 6 | 7,5866 | 0,0008 | 0,17 | 14NO2 GS |
| 6 | 2 | 4 | 5 | 2 | 4 | 5,0694 | 0,0002 | 0,56 | 14NO2 GS |
| 4 | 2 | 2 | 3 | 2 | 2 | 3,3766 | -0,0014 | 0,31 | 14NO2 GS |
| 3 | 2 | 2 | 2 | 2 | 0 | 2,5329 | 0,0000 | 0,31 | 14NO2 GS |
| 48 | 3 | 45 | 46 | 3 | 43 | 80,3439 | 0,0013 | 0,13 | 14NO2 GS |
| 47 | 3 | 45 | 45 | 3 | 43 | 78,4196 | 0,0195 | 0,10 | 14NO2 GS |
| 46 | 3 | 43 | 44 | 3 | 41 | 76,9545 | 0,0101 | 0,17 | 14NO2 GS |
| 45 | 3 | 43 | 43 | 3 | 41 | 75,0478 | 0,0009 | 0,24 | 14NO2 GS |
| 44 | 3 | 41 | 42 | 3 | 39 | 73,5426 | -0,0060 | 0,40 | 14NO2 GS |
| 41 | 3 | 39 | 39 | 3 | 37 | 68,3348 | 0,0044 | 0,58 | 14NO2 GS |
| 39 | 3 | 37 | 37 | 3 | 35 | 64,9669 | -0,0009 | 1,00 | 14NO2 GS |
| 33 | 3 | 31 | 31 | 3 | 29 | 54,8639 | -0,0021 | 0,82 | 14NO2 GS |
| 32 | 3 | 29 | 30 | 3 | 27 | 53,2184 | -0,0010 | 1,00 | 14NO2 GS |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 31 | 3 | 29 | 29 | 3 | 27 | 51,4914 | -0,0036 | 0,67 | 14NO2 GS |
| 30 | 3 | 27 | 28 | 3 | 25 | 49,8347 | -0,0023 | 0,82 | 14NO2 GS |
| 28 | 3 | 25 | 26 | 3 | 23 | 46,4554 | -0,0003 | 0,33 | 14NO2 GS |
| 27 | 3 | 25 | 25 | 3 | 23 | 44,7520 | 0,0032 | 0,82 | 14NO2 GS |
| 26 | 3 | 23 | 24 | 3 | 21 | 43,0756 | 0,0003 | 1,16 | 14NO2 GS |
| 23 | 3 | 21 | 21 | 3 | 19 | 37,9975 | -0,0010 | 0,58 | 14NO2 GS |
| 21 | 3 | 19 | 19 | 3 | 17 | 34,6269 | 0,0047 | 1,00 | 14NO2 GS |
| 8 | 3 | 5 | 6 | 3 | 3 | 12,6718 | 0,0038 | 0,70 | 14NO2 GS |
| 7 | 3 | 5 | 5 | 3 | 3 | 10,9786 | -0,0004 | 0,67 | 14NO2 GS |
| 6 | 3 | 3 | 4 | 3 | 1 | 9,2837 | -0,0062 | 0,18 | 14NO2 GS |
| 5 | 3 | 3 | 3 | 3 | 1 | 7,6099 | 0,0091 | 0,67 | 14NO2 GS |
| 13 | 3 | 11 | 12 | 3 | 9 | 10,9786 | 0,0003 | 0,17 | 14NO2 GS |
| 10 | 3 | 7 | 9 | 3 | 7 | 8,4404 | -0,0050 | 0,37 | 14NO2 GS |
| 9 | 3 | 7 | 8 | 3 | 5 | 7,6020 | 0,0013 | 0,67 | 14NO2 GS |
| 8 | 3 | 5 | 7 | 3 | 5 | 6,7560 | -0,0003 | 1,32 | 14NO2 GS |
| 7 | 3 | 5 | 6 | 3 | 3 | 5,9129 | 0,0012 | 1,66 | 14NO2 GS |
| 6 | 3 | 3 | 5 | 3 | 3 | 5,0677 | 0,0005 | 1,17 | 14NO2 GS |
| 5 | 3 | 3 | 4 | 3 | 1 | 4,2253 | 0,0026 | 1,49 | 14NO2 GS |
| 4 | 3 | 1 | 3 | 3 | 1 | 3,3769 | -0,0013 | 1,00 | 14NO2 GS |
| 47 | 4 | 44 | 45 | 4 | 42 | 78,4237 | -0,0101 | 0,10 | 14NO2 GS |
| 46 | 4 | 42 | 44 | 4 | 40 | 76,7564 | -0,0109 | 0,27 | 14NO2 GS |
| 43 | 4 | 40 | 41 | 4 | 38 | 71,7083 | -0,0007 | 0,17 | 14NO2 GS |
| 41 | 4 | 38 | 39 | 4 | 36 | 68,3525 | 0,0085 | 0,31 | 14NO2 GS |
| 39 | 4 | 36 | 37 | 4 | 34 | 64,9779 | 0,0005 | 0,18 | 14NO2 GS |
| 33 | 4 | 30 | 31 | 4 | 28 | 54,8657 | -0,0039 | 0,31 | 14NO2 GS |
| 31 | 4 | 28 | 29 | 4 | 26 | 51,4973 | -0,0007 | 0,52 | 14NO2 GS |
| 29 | 4 | 26 | 27 | 4 | 24 | 48,1213 | -0,0041 | 1,18 | 14NO2 GS |
| 23 | 4 | 20 | 21 | 4 | 18 | 37,9962 | -0,0061 | 0,82 | 14NO2 GS |
| 21 | 4 | 18 | 19 | 4 | 16 | 34,6321 | 0,0056 | 0,67 | 14NO2 GS |
| 18 | 4 | 14 | 16 | 4 | 12 | 29,5598 | -0,0019 | 0,82 | 14NO2 GS |
| 17 | 4 | 14 | 15 | 4 | 12 | 27,8676 | -0,0055 | 0,82 | 14NO2 GS |
| 15 | 4 | 12 | 13 | 4 | 10 | 24,4997 | 0,0040 | 0,29 | 14NO2 GS |
| 8 | 4 | 4 | 6 | 4 | 2 | 12,6703 | -0,0013 | 0,17 | 14NO2 GS |
| 6 | 4 | 2 | 4 | 4 | 0 | 9,2958 | 0,0031 | 0,13 | 14NO2 GS |
| 10 | 4 | 6 | 9 | 4 | 6 | 8,4533 | 0,0058 | 0,58 | 14NO2 GS |
| 8 | 4 | 4 | 7 | 4 | 4 | 6,7616 | 0,0035 | 0,18 | 14NO2 GS |
| 7 | 4 | 4 | 6 | 4 | 2 | 5,9100 | -0,0034 | 0,95 | 14NO2 GS |
| 36 | 5 | 31 | 34 | 5 | 29 | 59,9257 | -0,0032 | 0,70 | 14NO2 GS |
| 35 | 5 | 31 | 33 | 5 | 29 | 58,2382 | -0,0066 | 0,82 | 14NO2 GS |
| 33 | 5 | 29 | 31 | 5 | 27 | 54,8675 | -0,0080 | 1,17 | 14NO2 GS |
| 32 | 5 | 27 | 30 | 5 | 25 | 53,1837 | -0,0068 | 0,17 | 14NO2 GS |
| 28 | 5 | 23 | 26 | 5 | 21 | 46,4500 | 0,0031 | 0,46 | 14NO2 GS |
| 27 | 5 | 23 | 25 | 5 | 21 | 44,7667 | 0,0064 | 0,18 | 14NO2 GS |
| 25 | 5 | 21 | 23 | 5 | 19 | 41,3879 | 0,0015 | 0,46 | 14NO2 GS |
| 17 | 5 | 13 | 15 | 5 | 11 | 27,8812 | -0,0002 | 0,82 | 14NO2 GS |
| 17 | 5 | 13 | 16 | 5 | 11 | 14,3699 | 0,0070 | 1,00 | 14NO2 GS |
| 16 | 5 | 11 | 15 | 5 | 11 | 13,5160 | -0,0025 | 0,31 | 14NO2 GS |
| 13 | 5 | 9 | 12 | 5 | 7 | 10,9718 | -0,0129 | 0,15 | 14NO2 GS |
| 12 | 5 | 7 | 11 | 5 | 7 | 10,1411 | 0,0011 | 1,46 | 14NO2 GS |
| 11 | 5 | 7 | 10 | 5 | 5 | 9,2973 | 0,0021 | 1,00 | 14NO2 GS |
| 10 | 5 | 5 | 9 | 5 | 5 | 8,4478 | -0,0025 | 0,67 | 14NO2 GS |
| 9 | 5 | 5 | 8 | 5 | 3 | 7,6092 | 0,0038 | 0,67 | 14NO2 GS |
| 8 | 5 | 3 | 7 | 5 | 3 | 6,7624 | 0,0019 | 0,15 | 14NO2 GS |
| 37 | 6 | 32 | 35 | 6 | 30 | 61,6272 | 0,0013 | 0,58 | 14NO2 GS |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 34 | 6 | 28 | 32 | 6 | 26 | 56,5891 | 0,0150 | 0,17 | 14NO2 GS |
| 28 | 6 | 22 | 26 | 6 | 20 | 46,4587 | -0,0018 | 0,82 | 14NO2 GS |
| 26 | 6 | 20 | 24 | 6 | 18 | 43,0941 | 0,0075 | 0,50 | 14NO2 GS |
| 25 | 6 | 20 | 23 | 6 | 18 | 41,3913 | -0,0079 | 0,31 | 14NO2 GS |
| 23 | 6 | 18 | 21 | 6 | 16 | 38,0195 | -0,0042 | 0,58 | 14NO2 GS |
| 21 | 6 | 16 | 19 | 6 | 14 | 34,6531 | 0,0060 | 0,18 | 14NO2 GS |
| 20 | 6 | 14 | 18 | 6 | 12 | 32,9811 | 0,0226 | 0,18 | 14NO2 GS |
| 19 | 6 | 14 | 17 | 6 | 12 | 31,2713 | 0,0017 | 0,33 | 14NO2 GS |
| 18 | 6 | 12 | 16 | 6 | 10 | 29,5913 | 0,0107 | 0,30 | 14NO2 GS |
| 17 | 6 | 12 | 15 | 6 | 10 | 27,8988 | 0,0075 | 0,17 | 14NO2 GS |
| 20 | 6 | 14 | 19 | 6 | 14 | 16,9138 | 0,0124 | 0,18 | 14NO2 GS |
| 19 | 6 | 14 | 18 | 6 | 12 | 16,0579 | 0,0008 | 0,28 | 14NO2 GS |
| 18 | 6 | 12 | 17 | 6 | 12 | 15,2185 | 0,0059 | 0,13 | 14NO2 GS |
| 16 | 6 | 10 | 15 | 6 | 10 | 13,5280 | 0,0047 | 0,46 | 14NO2 GS |
| 14 | 6 | 8 | 13 | 6 | 8 | 11,8305 | -0,0032 | 0,82 | 14NO2 GS |
| 12 | 6 | 6 | 11 | 6 | 6 | 10,1333 | -0,0104 | 0,13 | 14NO2 GS |
| 9 | 6 | 4 | 8 | 6 | 2 | 7,6146 | 0,0063 | 0,24 | 14NO2 GS |
| 8 | 6 | 2 | 7 | 6 | 2 | 6,7746 | 0,0115 | 0,17 | 14NO2 GS |
| 16 | 7 | 9 | 15 | 7 | 9 | 13,5202 | -0,0080 | 0,18 | 14NO2 GS |
| 15 | 7 | 9 | 14 | 7 | 7 | 12,6808 | -0,0023 | 0,37 | 14NO2 GS |

## GROUND STATE COMBINATION DIFFERENCES FOR 15NO2

| UPPER | | | LOWER | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| N | K-1 | K+1 | N | K-1 | K+1 | OBSERVED | OBS-CALC | WEIGHT | |
| 3 | 1 | 3 | 4 | 0 | 4 | 3,762178 | 0,000008 | 25000 | 15 MICRO |
| 5 | 1 | 5 | 6 | 0 | 6 | 1,969932 | 0,000000 | 100000 | 15 MICRO |
| 7 | 1 | 7 | 8 | 0 | 8 | 0,133759 | -0,000016 | 25000 | 15 MICRO |
| 10 | 0 | 10 | 9 | 1 | 9 | 1,743318 | -0,000005 | 25000 | 15 MICRO |
| 12 | 0 | 12 | 11 | 1 | 11 | 3,657656 | -0,000000 | 250000 | 15 MICRO |
| 21 | 2 | 20 | 22 | 1 | 21 | 0,094008 | -0,000000 | 100000 | 15 MICRO |
| 46 | 0 | 46 | 44 | 0 | 44 | 75,2587 | -0,0150 | 0,13 | 15NO2 GS |
| 38 | 0 | 38 | 36 | 0 | 36 | 62,2784 | -0,0049 | 0,18 | 15NO2 GS |
| 36 | 0 | 36 | 34 | 0 | 34 | 59,0236 | -0,0032 | 0,18 | 15NO2 GS |
| 34 | 0 | 34 | 32 | 0 | 32 | 55,7663 | 0,0011 | 0,33 | 15NO2 GS |
| 32 | 0 | 32 | 30 | 0 | 30 | 52,4936 | -0,0039 | 0,67 | 15NO2 GS |
| 30 | 0 | 30 | 28 | 0 | 28 | 49,2237 | 0,0009 | 0,17 | 15NO2 GS |
| 28 | 0 | 28 | 26 | 0 | 26 | 45,9387 | -0,0015 | 0,63 | 15NO2 GS |
| 26 | 0 | 26 | 24 | 0 | 24 | 42,6465 | -0,0025 | 1,18 | 15NO2 GS |
| 24 | 0 | 24 | 22 | 0 | 22 | 39,3476 | -0,0011 | 2,00 | 15NO2 GS |
| 22 | 0 | 22 | 20 | 0 | 20 | 36,0398 | 0,0007 | 0,42 | 15NO2 GS |
| 20 | 0 | 20 | 18 | 0 | 18 | 32,7199 | -0,0002 | 2,00 | 15NO2 GS |
| 18 | 0 | 18 | 16 | 0 | 16 | 29,3914 | -0,0007 | 1,00 | 15NO2 GS |
| 16 | 0 | 16 | 14 | 0 | 14 | 26,0561 | 0,0007 | 1,00 | 15NO2 GS |
| 14 | 0 | 14 | 12 | 0 | 12 | 22,7131 | 0,0023 | 0,18 | 15NO2 GS |
| 6 | 0 | 6 | 4 | 0 | 4 | 9,2717 | 0,0002 | 0,13 | 15NO2 GS |
| 4 | 0 | 4 | 2 | 0 | 2 | 5,8942 | -0,0073 | 0,17 | 15NO2 GS |
| 48 | 1 | 47 | 46 | 1 | 45 | 80,2960 | 0,0132 | 0,13 | 15NO2 GS |
| 46 | 1 | 45 | 44 | 1 | 43 | 76,9902 | 0,0035 | 0,58 | 15NO2 GS |
| 45 | 1 | 45 | 43 | 1 | 43 | 73,4650 | 0,0002 | 0,42 | 15NO2 GS |
| 44 | 1 | 43 | 42 | 1 | 41 | 73,6845 | 0,0050 | 0,77 | 15NO2 GS |
| 42 | 1 | 41 | 40 | 1 | 39 | 70,3614 | -0,0000 | 1,13 | 15NO2 GS |
| 39 | 1 | 39 | 37 | 1 | 37 | 63,6451 | -0,0054 | 0,15 | 15NO2 GS |
| 37 | 1 | 37 | 35 | 1 | 35 | 60,3765 | 0,0046 | 0,67 | 15NO2 GS |
| 36 | 1 | 35 | 34 | 1 | 33 | 60,3457 | -0,0012 | 0,33 | 15NO2 GS |
| 35 | 1 | 35 | 33 | 1 | 33 | 57,0825 | -0,0072 | 0,50 | 15NO2 GS |
| 32 | 1 | 31 | 30 | 1 | 29 | 53,6166 | -0,0091 | 0,17 | 15NO2 GS |
| 30 | 1 | 29 | 28 | 1 | 27 | 50,2526 | -0,0009 | 1,00 | 15NO2 GS |
| 29 | 1 | 29 | 27 | 1 | 27 | 47,2187 | -0,0029 | 0,18 | 15NO2 GS |
| 28 | 1 | 27 | 26 | 1 | 25 | 46,8775 | 0,0031 | 0,79 | 15NO2 GS |
| 26 | 1 | 25 | 24 | 1 | 23 | 43,4875 | -0,0015 | 1,67 | 15NO2 GS |
| 25 | 1 | 25 | 23 | 1 | 23 | 40,6260 | 0,0007 | 1,18 | 15NO2 GS |
| 24 | 1 | 23 | 22 | 1 | 21 | 40,0961 | -0,0019 | 0,52 | 15NO2 GS |
| 16 | 1 | 15 | 14 | 1 | 13 | 26,4897 | 0,0019 | 0,46 | 15NO2 GS |
| 15 | 1 | 15 | 13 | 1 | 13 | 24,0812 | 0,0007 | 1,00 | 15NO2 GS |
| 14 | 1 | 13 | 12 | 1 | 11 | 23,0807 | 0,0043 | 0,33 | 15NO2 GS |
| 13 | 1 | 13 | 11 | 1 | 11 | 20,7612 | -0,0025 | 1,18 | 15NO2 GS |
| 11 | 1 | 11 | 9 | 1 | 9 | 17,4449 | 0,0000 | 1,33 | 15NO2 GS |
| 9 | 1 | 9 | 7 | 1 | 7 | 14,1248 | 0,0005 | 1,67 | 15NO2 GS |
| 7 | 1 | 7 | 5 | 1 | 5 | 10,8022 | -0,0001 | 1,00 | 15NO2 GS |
| 6 | 1 | 5 | 4 | 1 | 3 | 9,4021 | -0,0060 | 0,46 | 15NO2 GS |
| 5 | 1 | 5 | 3 | 1 | 3 | 7,4801 | 0,0008 | 0,64 | 15NO2 GS |
| 4 | 1 | 3 | 2 | 1 | 1 | 5,9925 | 0,0050 | 0,82 | 15NO2 GS |
| 3 | 1 | 3 | 1 | 1 | 1 | 4,1548 | -0,0006 | 0,46 | 15NO2 GS |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 9 | 1 | 9 | 8 | 1 | 7 | 6,6022 | -0,0008 | 0,10 | 15NO2 GS |
| 6 | 1 | 5 | 5 | 1 | 5 | 5,4903 | -0,0057 | 0,50 | 15NO2 GS |
| 4 | 1 | 3 | 3 | 1 | 3 | 3,5673 | 0,0002 | 0,13 | 15NO2 GS |
| 3 | 1 | 3 | 2 | 1 | 1 | 2,4195 | -0,0008 | 0,52 | 15NO2 GS |
| 2 | 1 | 1 | 1 | 1 | 1 | 1,7351 | 0,0000 | 0,82 | 15NO2 GS |
| 48 | 2 | 46 | 46 | 2 | 44 | 80,8419 | 0,0019 | 0,15 | 15NO2 GS |
| 47 | 2 | 46 | 45 | 2 | 44 | 77,8669 | -0,0035 | 0,15 | 15NO2 GS |
| 46 | 2 | 44 | 44 | 2 | 42 | 77,4346 | -0,0067 | 0,17 | 15NO2 GS |
| 45 | 2 | 44 | 43 | 2 | 42 | 74,5584 | -0,0058 | 0,10 | 15NO2 GS |
| 44 | 2 | 42 | 42 | 2 | 40 | 74,0391 | 0,0037 | 0,10 | 15NO2 GS |
| 43 | 2 | 42 | 41 | 2 | 40 | 71,2632 | 0,0105 | 0,15 | 15NO2 GS |
| 42 | 2 | 40 | 40 | 2 | 38 | 70,6230 | -0,0001 | 0,67 | 15NO2 GS |
| 41 | 2 | 40 | 39 | 2 | 38 | 67,9529 | 0,0168 | 0,24 | 15NO2 GS |
| 40 | 2 | 38 | 38 | 2 | 36 | 67,2039 | -0,0015 | 0,67 | 15NO2 GS |
| 39 | 2 | 38 | 37 | 2 | 36 | 64,6107 | -0,0039 | 0,17 | 15NO2 GS |
| 38 | 2 | 36 | 36 | 2 | 34 | 63,7743 | -0,0090 | 0,15 | 15NO2 GS |
| 36 | 2 | 34 | 34 | 2 | 32 | 60,3588 | 0,0006 | 1,00 | 15NO2 GS |
| 33 | 2 | 32 | 31 | 2 | 30 | 54,6149 | -0,0069 | 0,10 | 15NO2 GS |
| 30 | 2 | 28 | 28 | 2 | 26 | 50,0706 | -0,0068 | 0,17 | 15NO2 GS |
| 29 | 2 | 28 | 27 | 2 | 26 | 47,9452 | 0,0069 | 0,18 | 15NO2 GS |
| 28 | 2 | 26 | 26 | 2 | 24 | 46,6609 | 0,0079 | 0,24 | 15NO2 GS |
| 26 | 2 | 24 | 24 | 2 | 22 | 43,2292 | -0,0028 | 0,67 | 15NO2 GS |
| 24 | 2 | 22 | 22 | 2 | 20 | 39,8094 | -0,0057 | 1,18 | 15NO2 GS |
| 22 | 2 | 20 | 20 | 2 | 18 | 36,4055 | 0,0025 | 0,18 | 15NO2 GS |
| 20 | 2 | 18 | 18 | 2 | 16 | 32,9953 | -0,0007 | 0,82 | 15NO2 GS |
| 18 | 2 | 16 | 16 | 2 | 14 | 29,5931 | -0,0013 | 1,37 | 15NO2 GS |
| 16 | 2 | 14 | 14 | 2 | 12 | 26,2038 | 0,0057 | 0,56 | 15NO2 GS |
| 5 | 2 | 4 | 3 | 2 | 2 | 7,5885 | -0,0012 | 1,00 | 15NO2 GS |
| 4 | 2 | 2 | 2 | 2 | 0 | 5,8954 | -0,0087 | 0,18 | 15NO2 GS |
| 7 | 2 | 6 | 6 | 2 | 4 | 5,8992 | 0,0010 | 0,37 | 15NO2 GS |
| 6 | 2 | 4 | 5 | 2 | 4 | 5,0650 | 0,0011 | 0,67 | 15NO2 GS |
| 5 | 2 | 4 | 4 | 2 | 2 | 4,2161 | 0,0006 | 2,00 | 15NO2 GS |
| 4 | 2 | 2 | 3 | 2 | 2 | 3,3719 | -0,0023 | 1,17 | 15NO2 GS |
| 3 | 2 | 2 | 2 | 2 | 0 | 2,5291 | -0,0009 | 1,17 | 15NO2 GS |
| 47 | 3 | 45 | 45 | 3 | 43 | 78,3217 | 0,0071 | 0,37 | 15NO2 GS |
| 44 | 3 | 41 | 42 | 3 | 39 | 73,4959 | -0,0171 | 0,13 | 15NO2 GS |
| 42 | 3 | 39 | 40 | 3 | 37 | 70,1059 | -0,0098 | 0,37 | 15NO2 GS |
| 39 | 3 | 37 | 37 | 3 | 35 | 64,8986 | -0,0002 | 0,60 | 15NO2 GS |
| 35 | 3 | 33 | 33 | 3 | 31 | 58,1764 | 0,0029 | 0,80 | 15NO2 GS |
| 34 | 3 | 31 | 32 | 3 | 29 | 56,5549 | -0,0012 | 0,35 | 15NO2 GS |
| 33 | 3 | 31 | 31 | 3 | 29 | 54,8031 | -0,0045 | 0,46 | 15NO2 GS |
| 29 | 3 | 27 | 27 | 3 | 25 | 48,0833 | 0,0126 | 0,10 | 15NO2 GS |
| 27 | 3 | 25 | 25 | 3 | 23 | 44,6968 | -0,0034 | 0,17 | 15NO2 GS |
| 26 | 3 | 23 | 24 | 3 | 21 | 43,0209 | -0,0109 | 0,15 | 15NO2 GS |
| 25 | 3 | 23 | 23 | 3 | 21 | 41,3276 | -0,0012 | 0,25 | 15NO2 GS |
| 24 | 3 | 21 | 22 | 3 | 19 | 39,6360 | -0,0182 | 0,10 | 15NO2 GS |
| 23 | 3 | 21 | 21 | 3 | 19 | 37,9539 | -0,0026 | 0,28 | 15NO2 GS |
| 21 | 3 | 19 | 19 | 3 | 17 | 34,5844 | 0,0008 | 0,18 | 15NO2 GS |
| 20 | 3 | 17 | 18 | 3 | 15 | 32,8959 | -0,0056 | 0,18 | 15NO2 GS |
| 19 | 3 | 17 | 17 | 3 | 15 | 31,2162 | 0,0060 | 1,17 | 15NO2 GS |
| 18 | 3 | 15 | 16 | 3 | 13 | 29,5296 | 0,0035 | 0,18 | 15NO2 GS |
| 15 | 3 | 13 | 13 | 3 | 11 | 24,4647 | 0,0021 | 0,18 | 15NO2 GS |
| 14 | 3 | 11 | 12 | 3 | 9 | 22,7772 | 0,0009 | 1,00 | 15NO2 GS |
| 13 | 3 | 11 | 11 | 3 | 9 | 21,0902 | 0,0017 | 1,00 | 15NO2 GS |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | 3 | 9 | 10 | 3 | 7 | 19,4000 | -0,0018 | 0,33 | 15NO2 | GS |
| 11 | 3 | 9 | 9 | 3 | 7 | 17,7164 | 0,0020 | 0,18 | 15NO2 | GS |
| 10 | 3 | 7 | 8 | 3 | 5 | 16,0296 | 0,0022 | 0,37 | 15NO2 | GS |
| 6 | 3 | 3 | 4 | 3 | 1 | 9,2838 | 0,0049 | 0,67 | 15NO2 | GS |
| 10 | 3 | 7 | 9 | 3 | 7 | 8,4355 | -0,0001 | 0,15 | 15NO2 | GS |
| 9 | 3 | 7 | 8 | 3 | 5 | 7,5955 | 0,0037 | 0,59 | 15NO2 | GS |
| 8 | 3 | 5 | 7 | 3 | 5 | 6,7475 | -0,0009 | 0,33 | 15NO2 | GS |
| 7 | 3 | 5 | 6 | 3 | 3 | 5,9063 | 0,0015 | 0,77 | 15NO2 | GS |
| 5 | 3 | 3 | 4 | 3 | 1 | 4,2230 | 0,0053 | 0,67 | 15NO2 | GS |
| 4 | 3 | 1 | 3 | 3 | 1 | 3,3817 | 0,0075 | 1,00 | 15NO2 | GS |
| 44 | 4 | 40 | 42 | 4 | 38 | 73,3293 | -0,0014 | 0,37 | 15NO2 | GS |
| 35 | 4 | 32 | 33 | 4 | 30 | 58,1761 | -0,0013 | 1,17 | 15NO2 | GS |
| 34 | 4 | 30 | 32 | 4 | 28 | 56,4955 | -0,0006 | 1,17 | 15NO2 | GS |
| 33 | 4 | 30 | 31 | 4 | 28 | 54,8117 | 0,0020 | 1,10 | 15NO2 | GS |
| 32 | 4 | 28 | 30 | 4 | 26 | 53,1289 | 0,0018 | 0,46 | 15NO2 | GS |
| 31 | 4 | 28 | 29 | 4 | 26 | 51,4500 | 0,0089 | 0,13 | 15NO2 | GS |
| 28 | 4 | 24 | 26 | 4 | 22 | 46,3886 | 0,0014 | 1,00 | 15NO2 | GS |
| 27 | 4 | 24 | 25 | 4 | 22 | 44,7043 | 0,0030 | 0,79 | 15NO2 | GS |
| 26 | 4 | 22 | 24 | 4 | 20 | 43,0222 | 0,0059 | 1,00 | 15NO2 | GS |
| 24 | 4 | 20 | 22 | 4 | 18 | 39,6519 | 0,0071 | 0,46 | 15NO2 | GS |
| 19 | 4 | 16 | 17 | 4 | 14 | 31,2119 | -0,0017 | 0,17 | 15NO2 | GS |
| 18 | 4 | 14 | 16 | 4 | 12 | 29,5202 | -0,0069 | 0,18 | 15NO2 | GS |
| 17 | 4 | 14 | 15 | 4 | 12 | 27,8309 | -0,0094 | 0,17 | 15NO2 | GS |
| 16 | 4 | 12 | 14 | 4 | 10 | 26,1556 | 0,0020 | 0,13 | 15NO2 | GS |
| 12 | 4 | 8 | 10 | 4 | 6 | 19,4122 | 0,0067 | 0,30 | 15NO2 | GS |
| 10 | 4 | 6 | 8 | 4 | 4 | 16,0118 | -0,0192 | 0,17 | 15NO2 | GS |
| 9 | 4 | 6 | 7 | 4 | 4 | 14,3403 | -0,0034 | 0,10 | 15NO2 | GS |
| 11 | 4 | 8 | 10 | 4 | 6 | 9,2830 | 0,0020 | 0,24 | 15NO2 | GS |
| 10 | 4 | 6 | 9 | 4 | 6 | 8,4340 | -0,0033 | 0,87 | 15NO2 | GS |
| 9 | 4 | 6 | 8 | 4 | 4 | 7,5749 | -0,0188 | 0,13 | 15NO2 | GS |
| 7 | 4 | 4 | 6 | 4 | 2 | 5,9121 | 0,0058 | 0,37 | 15NO2 | GS |
| 5 | 4 | 2 | 4 | 4 | 0 | 4,2306 | 0,0117 | 0,50 | 15NO2 | GS |
| 38 | 5 | 33 | 36 | 5 | 31 | 63,2240 | -0,0027 | 0,46 | 15NO2 | GS |
| 35 | 5 | 31 | 33 | 5 | 29 | 58,1675 | -0,0126 | 0,18 | 15NO2 | GS |
| 34 | 5 | 29 | 32 | 5 | 27 | 56,5108 | 0,0135 | 0,18 | 15NO2 | GS |
| 24 | 5 | 19 | 22 | 5 | 17 | 39,6527 | -0,0004 | 0,17 | 15NO2 | GS |
| 22 | 5 | 17 | 20 | 5 | 15 | 36,2845 | 0,0032 | 0,46 | 15NO2 | GS |
| 21 | 5 | 17 | 19 | 5 | 15 | 34,5949 | -0,0002 | 0,46 | 15NO2 | GS |
| 20 | 5 | 15 | 18 | 5 | 13 | 32,9043 | -0,0045 | 0,82 | 15NO2 | GS |
| 19 | 5 | 15 | 17 | 5 | 13 | 31,2178 | -0,0044 | 0,46 | 15NO2 | GS |
| 18 | 5 | 13 | 16 | 5 | 11 | 29,5367 | 0,0012 | 0,82 | 15NO2 | GS |
| 15 | 5 | 11 | 13 | 5 | 9 | 24,4727 | -0,0017 | 0,37 | 15NO2 | GS |
| 15 | 5 | 11 | 14 | 5 | 9 | 12,6530 | -0,0060 | 0,15 | 15NO2 | GS |
| 14 | 5 | 9 | 13 | 5 | 9 | 11,8178 | 0,0024 | 0,10 | 15NO2 | GS |
| 13 | 5 | 9 | 12 | 5 | 7 | 10,9739 | 0,0022 | 0,18 | 15NO2 | GS |
| 12 | 5 | 7 | 11 | 5 | 7 | 10,1237 | -0,0042 | 0,30 | 15NO2 | GS |
| 11 | 5 | 7 | 10 | 5 | 5 | 9,2845 | 0,0004 | 0,35 | 15NO2 | GS |
| 9 | 5 | 5 | 8 | 5 | 3 | 7,6007 | 0,0043 | 0,50 | 15NO2 | GS |
| 34 | 6 | 28 | 32 | 6 | 26 | 56,5071 | -0,0064 | 0,18 | 15NO2 | GS |
| 18 | 6 | 12 | 16 | 6 | 10 | 29,5279 | -0,0198 | 0,15 | 15NO2 | GS |
| 15 | 6 | 10 | 13 | 6 | 8 | 24,4927 | 0,0078 | 0,50 | 15NO2 | GS |
| 16 | 6 | 10 | 15 | 6 | 10 | 13,5008 | -0,0075 | 0,17 | 15NO2 | GS |

## APPENDIX III

### FREQUENCIES FOR THE (1,0,1) BAND OF $^{14}NO_2$

| | K | N | OBS | O-C | WT | | K | N | OBS | O-C | WT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| P | 0 | 48 | 2854,019 | -0,008 | 0,1 | P | 0 | 46 | 2856,669 | -0,005 | 0,2 |
| P | 0 | 44 | 2859,289 | 0,009 | 0,1 | P | 0 | 42 | 2861,819 | -0,022 | 0,1 |
| P | 0 | 40 | 2864,373 | 0,013 | 0,0 | P | 0 | 38 | 2866,834 | -0,003 | 0,1 |
| P | 0 | 36 | 2869,246 | -0,026 | 0,0 | P | 0 | 34 | 2871,665 | 0,001 | 0,7 |
| P | 0 | 32 | 2874,016 | 0,003 | 1,0 | P | 0 | 30 | 2876,323 | 0,002 | 1,0 |
| P | 0 | 28 | 2878,592 | 0,004 | 1,0 | P | 0 | 26 | 2880,815 | 0,001 | 1,0 |
| P | 0 | 24 | 2883,002 | 0,003 | 1,0 | P | 0 | 22 | 2885,130 | -0,012 | 0,0 |
| P | 0 | 20 | 2887,247 | -0,000 | 0,3 | P | 0 | 18 | 2889,311 | 0,001 | 1,0 |
| P | 0 | 16 | 2891,334 | -0,000 | 0,7 | P | 0 | 14 | 2893,316 | -0,003 | 1,0 |
| P | 0 | 12 | 2895,265 | 0,003 | 0,7 | P | 0 | 10 | 2897,170 | 0,004 | 1,0 |
| P | 0 | 8 | 2899,033 | 0,004 | 0,7 | P | 0 | 6 | 2900,863 | 0,010 | 0,7 |
| P | 0 | 4 | 2902,639 | 0,005 | 0,0 | P | 0 | 2 | 2904,382 | 0,007 | 0,1 |
| P | 1 | 48 | 2853,423 | -0,005 | 0,1 | P | 1 | 47 | 2855,340 | -0,006 | 0,2 |
| P | 1 | 46 | 2856,074 | -0,006 | 0,3 | P | 1 | 45 | 2857,966 | -0,007 | 0,2 |
| P | 1 | 44 | 2858,688 | -0,004 | 0,5 | P | 1 | 43 | 2860,560 | 0,002 | 0,1 |
| P | 1 | 42 | 2861,264 | 0,003 | 0,7 | P | 1 | 41 | 2863,100 | -0,001 | 0,0 |
| P | 1 | 40 | 2863,793 | 0,002 | 0,0 | P | 1 | 39 | 2865,608 | 0,005 | 0,2 |
| P | 1 | 38 | 2866,279 | -0,001 | 0,7 | P | 1 | 37 | 2868,056 | -0,006 | 0,2 |
| P | 1 | 36 | 2868,727 | -0,001 | 0,5 | P | 1 | 35 | 2870,484 | 0,006 | 0,7 |
| P | 1 | 34 | 2871,136 | -0,001 | 1,0 | P | 1 | 33 | 2872,851 | -0,001 | 1,0 |
| P | 1 | 32 | 2873,500 | -0,006 | 1,0 | P | 1 | 31 | 2875,182 | -0,002 | 0,7 |
| P | 1 | 30 | 2875,835 | 0,001 | 1,0 | P | 1 | 29 | 2877,473 | -0,001 | 1,0 |
| P | 1 | 28 | 2878,124 | 0,002 | 1,0 | P | 1 | 27 | 2879,724 | 0,003 | 0,7 |
| P | 1 | 26 | 2880,383 | 0,013 | 0,0 | P | 1 | 25 | 2881,926 | -0,001 | 1,0 |
| P | 1 | 24 | 2882,564 | -0,014 | 0,0 | P | 1 | 23 | 2884,098 | 0,008 | 0,1 |
| P | 1 | 22 | 2884,746 | -0,000 | 1,0 | P | 1 | 21 | 2886,212 | 0,001 | 0,7 |
| P | 1 | 20 | 2886,876 | 0,002 | 1,0 | P | 1 | 19 | 2888,291 | 0,001 | 0,7 |
| P | 1 | 18 | 2888,991 | 0,029 | 0,0 | P | 1 | 17 | 2890,327 | -0,000 | 1,0 |
| P | 1 | 16 | 2891,006 | -0,004 | 0,0 | P | 1 | 15 | 2892,325 | 0,003 | 1,0 |
| P | 1 | 14 | 2893,002 | -0,015 | 0,0 | P | 1 | 13 | 2894,277 | 0,003 | 1,0 |
| P | 1 | 12 | 2894,981 | -0,003 | 1,0 | P | 1 | 11 | 2896,193 | 0,009 | 0,1 |
| P | 1 | 10 | 2896,908 | -0,002 | 0,7 | P | 1 | 9 | 2898,052 | -0,001 | 1,0 |
| P | 1 | 8 | 2898,793 | -0,003 | 1,0 | P | 1 | 7 | 2899,878 | 0,001 | 0,7 |
| P | 1 | 6 | 2900,643 | 0,002 | 0,0 | P | 1 | 5 | 2901,662 | 0,002 | 0,1 |
| P | 1 | 4 | 2902,446 | 0,000 | 0,7 | P | 1 | 3 | 2903,401 | 0,001 | 0,0 |
| P | 1 | 2 | 2904,202 | -0,006 | 0,0 | P | 2 | 48 | 2853,016 | -0,011 | 0,1 |
| P | 2 | 47 | 2854,606 | 0,004 | 0,1 | P | 2 | 46 | 2855,669 | -0,015 | 0,1 |
| P | 2 | 45 | 2857,230 | -0,002 | 0,1 | P | 2 | 44 | 2858,296 | -0,006 | 0,7 |
| P | 2 | 43 | 2859,808 | -0,014 | 0,7 | P | 2 | 42 | 2860,874 | -0,007 | 0,5 |
| P | 2 | 41 | 2862,367 | -0,002 | 0,1 | P | 2 | 40 | 2863,415 | -0,005 | 0,5 |
| P | 2 | 39 | 2864,874 | -0,002 | 0,7 | P | 2 | 38 | 2865,918 | -0,000 | 0,2 |
| P | 2 | 37 | 2867,333 | -0,008 | 0,2 | P | 2 | 36 | 2868,376 | -0,001 | 1,0 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| P | 2 | 35 | 2869,762 | -0,003 | 1,0 | P | 2 | 34 | 2870,795 | -0,001 | 1,0 |
| P | 2 | 33 | 2872,155 | 0,008 | 0,0 | P | 2 | 32 | 2873,170 | -0,005 | 0,7 |
| P | 2 | 31 | 2874,471 | -0,018 | 0,0 | P | 2 | 30 | 2875,517 | 0,004 | 0,2 |
| P | 2 | 29 | 2876,789 | 0,000 | 1,0 | P | 2 | 28 | 2877,800 | -0,010 | 0,5 |
| P | 2 | 27 | 2879,053 | 0,005 | 0,2 | P | 2 | 26 | 2880,065 | -0,000 | 1,0 |
| P | 2 | 25 | 2881,266 | -0,000 | 0,0 | P | 2 | 24 | 2882,264 | -0,015 | 0,0 |
| P | 2 | 23 | 2883,440 | -0,003 | 1,0 | P | 2 | 22 | 2884,450 | -0,001 | 1,0 |
| P | 2 | 21 | 2885,575 | -0,003 | 1,0 | P | 2 | 20 | 2886,579 | -0,000 | 1,0 |
| P | 2 | 19 | 2887,692 | 0,019 | 0,0 | P | 2 | 18 | 2888,667 | 0,002 | 0,0 |
| P | 2 | 17 | 2889,709 | -0,017 | 0,0 | P | 2 | 16 | 2890,691 | -0,016 | 0,0 |
| P | 2 | 15 | 2891,735 | -0,003 | 1,0 | P | 2 | 14 | 2892,703 | -0,005 | 1,0 |
| P | 2 | 13 | 2893,707 | -0,001 | 1,0 | P | 2 | 12 | 2894,662 | -0,002 | 1,0 |
| P | 2 | 11 | 2895,636 | -0,001 | 0,7 | P | 2 | 10 | 2896,573 | -0,005 | 0,7 |
| P | 2 | 9 | 2897,523 | -0,001 | 0,7 | P | 2 | 8 | 2898,457 | 0,009 | 0,0 |
| P | 2 | 7 | 2899,366 | -0,004 | 0,0 | P | 2 | 6 | 2900,278 | 0,003 | 0,1 |
| P | 2 | 5 | 2901,166 | -0,007 | 0,0 | P | 2 | 4 | 2902,068 | 0,009 | 0,0 |
| P | 2 | 3 | 2902,940 | 0,004 | 0,0 | P | 3 | 48 | 2852,455 | -0,001 | 0,0 |
| P | 3 | 47 | 2853,815 | -0,011 | 0,1 | P | 3 | 46 | 2855,093 | -0,019 | 0,1 |
| P | 3 | 45 | 2856,446 | -0,011 | 0,0 | P | 3 | 44 | 2857,723 | -0,003 | 0,1 |
| P | 3 | 43 | 2859,044 | -0,004 | 0,0 | P | 3 | 42 | 2860,293 | -0,008 | 0,0 |
| P | 3 | 41 | 2861,595 | -0,003 | 0,7 | P | 3 | 40 | 2862,827 | -0,007 | 0,7 |
| P | 3 | 39 | 2864,104 | -0,004 | 1,0 | P | 3 | 38 | 2865,323 | -0,003 | 0,7 |
| P | 3 | 37 | 2866,372 | -0,004 | 0,5 | P | 3 | 36 | 2867,776 | -0,001 | 0,5 |
| P | 3 | 35 | 2869,007 | 0,004 | 1,0 | P | 3 | 34 | 2870,187 | -0,001 | 0,7 |
| P | 3 | 33 | 2871,395 | 0,005 | 0,1 | P | 3 | 32 | 2872,563 | 0,006 | 0,0 |
| P | 3 | 31 | 2873,734 | -0,001 | 0,0 | P | 3 | 30 | 2874,878 | -0,006 | 0,0 |
| P | 3 | 29 | 2876,026 | -0,014 | 0,0 | P | 3 | 28 | 2877,165 | -0,005 | 0,2 |
| P | 3 | 27 | 2878,299 | -0,004 | 0,7 | P | 3 | 26 | 2879,409 | -0,005 | 1,0 |
| P | 3 | 25 | 2880,522 | -0,003 | 1,0 | P | 3 | 24 | 2881,614 | -0,003 | 1,0 |
| P | 3 | 23 | 2882,705 | -0,001 | 0,7 | P | 3 | 22 | 2883,777 | -0,000 | 1,0 |
| P | 3 | 21 | 2884,838 | -0,006 | 1,0 | P | 3 | 20 | 2885,904 | 0,007 | 0,1 |
| P | 3 | 19 | 2886,956 | 0,014 | 0,0 | P | 3 | 18 | 2887,983 | 0,010 | 0,0 |
| P | 3 | 17 | 2888,994 | -0,003 | 0,0 | P | 3 | 16 | 2890,004 | -0,005 | 0,3 |
| P | 3 | 15 | 2891,006 | -0,005 | 0,0 | P | 3 | 14 | 2891,983 | -0,019 | 0,0 |
| P | 3 | 13 | 2892,997 | 0,014 | 0,0 | P | 3 | 12 | 2893,944 | -0,010 | 0,0 |
| P | 3 | 11 | 2894,909 | -0,005 | 0,5 | P | 3 | 10 | 2895,857 | -0,007 | 0,3 |
| P | 3 | 9 | 2896,795 | -0,007 | 0,5 | P | 3 | 8 | 2897,727 | -0,004 | 0,5 |
| P | 3 | 7 | 2898,652 | 0,003 | 0,1 | P | 3 | 6 | 2899,556 | -0,001 | 0,2 |
| P | 3 | 5 | 2900,459 | 0,005 | 0,0 | P | 3 | 4 | 2901,340 | -0,000 | 0,0 |
| P | 4 | 48 | 2851,581 | 0,068 | 0,0 | P | 4 | 47 | 2852,922 | 0,076 | 0,0 |
| P | 4 | 46 | 2854,225 | 0,062 | 0,1 | P | 4 | 45 | 2855,532 | 0,058 | 0,1 |
| P | 4 | 44 | 2856,824 | 0,052 | 0,1 | P | 4 | 43 | 2858,110 | 0,047 | 0,1 |
| P | 4 | 42 | 2859,383 | 0,042 | 0,1 | P | 4 | 41 | 2860,648 | 0,036 | 0,2 |
| P | 4 | 40 | 2861,903 | 0,034 | 0,3 | P | 4 | 39 | 2863,156 | 0,038 | 0,1 |
| P | 4 | 38 | 2864,373 | 0,017 | 0,0 | P | 4 | 37 | 2865,608 | 0,022 | 0,0 |
| P | 4 | 36 | 2866,834 | 0,032 | 0,0 | P | 4 | 35 | 2868,056 | 0,045 | 0,0 |
| P | 4 | 34 | 2869,243 | 0,034 | 0,0 | P | 4 | 33 | 2870,421 | 0,025 | 0,7 |
| P | 4 | 32 | 2871,596 | 0,024 | 0,5 | P | 4 | 31 | 2872,755 | 0,016 | 0,2 |
| P | 4 | 30 | 2873,911 | 0,015 | 0,2 | P | 4 | 29 | 2875,062 | 0,020 | 1,0 |
| P | 4 | 28 | 2876,193 | 0,015 | 1,0 | P | 4 | 27 | 2877,316 | 0,013 | 1,0 |
| P | 4 | 26 | 2878,431 | 0,012 | 1,0 | P | 4 | 25 | 2879,532 | 0,008 | 1,0 |
| P | 4 | 24 | 2880,624 | 0,005 | 1,0 | P | 4 | 23 | 2881,712 | 0,010 | 1,0 |
| P | 4 | 22 | 2882,781 | 0,005 | 1,0 | P | 4 | 21 | 2883,844 | 0,004 | 1,0 |
| P | 4 | 20 | 2884,896 | 0,003 | 1,0 | P | 4 | 19 | 2885,941 | 0,004 | 0,1 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| P | 4 | 18 | 2886,956 | -0,013 | 0,0 | P | 4 | 17 | 2887,983 | -0.007 | 0,0 |
| P | 4 | 16 | 2888,994 | -0,009 | 0,0 | P | 4 | 15 | 2890,004 | 0.001 | 0,2 |
| P | 4 | 14 | 2891,006 | 0,011 | 0,0 | P | 4 | 13 | 2891,983 | 0.008 | 0,0 |
| P | 4 | 12 | 2892,958 | 0,013 | 0,0 | P | 4 | 11 | 2893,909 | 0.004 | 0,0 |
| P | 4 | 10 | 2894,856 | 0,001 | 0,7 | P | 4 | 9 | 2895,792 | -0.001 | 0,2 |
| P | 4 | 8 | 2896,721 | -0,000 | 0,0 | P | 4 | 7 | 2897,648 | 0.009 | 0,0 |
| P | 4 | 6 | 2898,545 | -0,002 | 0,2 | P | 4 | 5 | 2899,442 | -0.002 | 0,0 |
| P | 5 | 48 | 2850,233 | -0,027 | 0,0 | P | 5 | 47 | 2851,534 | -0,055 | 0,0 |
| P | 5 | 46 | 2852,871 | -0,036 | 0,1 | P | 5 | 45 | 2854,163 | -0,051 | 0,1 |
| P | 5 | 44 | 2855,475 | -0,036 | 0,1 | P | 5 | 43 | 2856,753 | -0,046 | 0,0 |
| P | 5 | 42 | 2858,040 | -0,036 | 0,1 | P | 5 | 41 | 2859,289 | -0,055 | 0,1 |
| P | 5 | 40 | 2860,560 | -0,041 | 0,1 | P | 5 | 39 | 2861,819 | -0,028 | 0,1 |
| P | 5 | 38 | 2863,049 | -0,035 | 0,0 | P | 5 | 37 | 2864,285 | -0,027 | 0,2 |
| P | 5 | 36 | 2865,509 | -0,018 | 0,7 | P | 5 | 35 | 2866,720 | -0,014 | 0,7 |
| P | 5 | 34 | 2867,918 | -0,012 | 0,7 | P | 5 | 33 | 2869,098 | -0,017 | 0,7 |
| P | 5 | 32 | 2870,273 | -0,018 | 0,7 | P | 5 | 31 | 2871,435 | -0,021 | 0,0 |
| P | 5 | 30 | 2872,601 | -0,011 | 0,0 | P | 5 | 29 | 2873,734 | -0,023 | 0,0 |
| P | 5 | 28 | 2874,878 | -0,013 | 0,0 | P | 5 | 27 | 2876,026 | 0.010 | 0,0 |
| P | 5 | 26 | 2877,127 | -0,003 | 0,1 | P | 5 | 25 | 2878,223 | -0,011 | 0,7 |
| P | 5 | 24 | 2879,320 | -0,008 | 1,0 | P | 5 | 23 | 2880,383 | -0,028 | 0,0 |
| P | 5 | 22 | 2881,479 | -0,004 | 1,0 | P | 5 | 21 | 2882,564 | 0.017 | 0,0 |
| P | 5 | 20 | 2883,598 | -0,001 | 1,0 | P | 5 | 19 | 2884,637 | -0,004 | 1,0 |
| P | 5 | 18 | 2885,667 | -0,006 | 1,0 | P | 5 | 17 | 2886,693 | -0,002 | 1,0 |
| P | 5 | 16 | 2887,693 | -0,012 | 0,0 | P | 5 | 15 | 2888,697 | -0,010 | 0,0 |
| P | 5 | 14 | 2889,709 | 0,012 | 0,0 | P | 5 | 13 | 2890,689 | 0,012 | 0,0 |
| P | 5 | 12 | 2891,644 | -0,003 | 1,0 | P | 5 | 11 | 2892,606 | -0.001 | 1,0 |
| P | 5 | 10 | 2893,568 | 0,012 | 0,1 | P | 5 | 9 | 2894,504 | 0.009 | 0,0 |
| P | 5 | 8 | 2895,424 | 0,001 | 0,0 | P | 5 | 7 | 2896,336 | -0,005 | 0,0 |
| P | 5 | 6 | 2897,239 | -0,009 | 0,1 | P | 6 | 41 | 2857,780 | -0,016 | 0,1 |
| P | 6 | 40 | 2859,044 | -0,007 | 0,0 | P | 6 | 39 | 2860,293 | -0,003 | 0,0 |
| P | 6 | 38 | 2861,524 | -0,007 | 0,2 | P | 6 | 37 | 2862,752 | -0,003 | 0,5 |
| P | 6 | 36 | 2863,964 | -0,006 | 0,5 | P | 6 | 35 | 2865,171 | -0,004 | 0,5 |
| P | 6 | 34 | 2866,357 | -0,012 | 0,5 | P | 6 | 33 | 2867,551 | -0,002 | 0,5 |
| P | 6 | 32 | 2868,727 | 0,000 | 0,0 | P | 6 | 31 | 2869,883 | -0,008 | 0,5 |
| P | 6 | 30 | 2871,045 | 0,001 | 0,5 | P | 6 | 29 | 2872,189 | 0.001 | 0,0 |
| P | 6 | 28 | 2873,324 | 0,002 | 1,0 | P | 6 | 27 | 2874,471 | 0.026 | 0,0 |
| P | 6 | 26 | 2875,557 | -0,000 | 0,5 | P | 6 | 25 | 2876,673 | 0.012 | 0,2 |
| P | 6 | 24 | 2877,759 | 0,006 | 0,5 | P | 6 | 23 | 2878,838 | 0.002 | 1,0 |
| P | 6 | 22 | 2879,894 | -0,013 | 1,0 | P | 6 | 21 | 2880,972 | 0.003 | 1,0 |
| P | 6 | 20 | 2882,021 | -0,000 | 1,0 | P | 6 | 19 | 2883,067 | 0.005 | 1,0 |
| P | 6 | 18 | 2884,098 | 0,004 | 0,0 | P | 6 | 17 | 2885,130 | 0.016 | 0,0 |
| P | 6 | 16 | 2886,126 | 0,001 | 1,0 | P | 6 | 15 | 2887,129 | 0.003 | 1,0 |
| P | 6 | 14 | 2888,122 | 0,007 | 1,0 | P | 6 | 13 | 2889,103 | 0.008 | 0,0 |
| P | 6 | 12 | 2890,071 | 0,006 | 0,1 | P | 6 | 11 | 2891,006 | -0.017 | 0,0 |
| P | 6 | 10 | 2891,984 | 0,011 | 0,0 | P | 6 | 9 | 2892,928 | 0.017 | 0,0 |
| P | 6 | 8 | 2893,852 | 0,013 | 0,0 | P | 6 | 7 | 2894,758 | 0.001 | 0,0 |
| P | 7 | 40 | 2857,230 | -0,003 | 0,0 | P | 7 | 39 | 2858,481 | 0.006 | 0,1 |
| P | 7 | 38 | 2859,719 | 0,010 | 0,2 | P | 7 | 37 | 2860,944 | 0.013 | 0,5 |
| P | 7 | 36 | 2862,157 | 0,013 | 0,0 | P | 7 | 35 | 2863,353 | 0.006 | 0,5 |
| P | 7 | 34 | 2864,553 | 0,014 | 0,1 | P | 7 | 33 | 2865,740 | 0.019 | 0,0 |
| P | 7 | 32 | 2866,900 | 0,007 | 0,7 | P | 7 | 31 | 2868,055 | -0.001 | 0,0 |
| P | 7 | 30 | 2869,248 | 0,041 | 0,0 | P | 7 | 29 | 2870,350 | -0.000 | 0,5 |
| P | 7 | 28 | 2871,497 | 0,015 | 0,0 | P | 7 | 27 | 2872,598 | -0.005 | 0,0 |
| P | 7 | 26 | 2873,739 | 0,021 | 0,0 | P | 7 | 25 | 2874,824 | 0.008 | 0,1 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| P | 7 | 24 | 2875,925 | 0,018 | 0,1 | P | 7 | 23 | 2876,997 | 0,008 | 1,0 |
| P | 7 | 22 | 2878,061 | 0,002 | 0,3 | P | 7 | 21 | 2879,113 | -0,007 | 0,1 |
| P | 7 | 20 | 2880,176 | 0,005 | 0,7 | P | 7 | 19 | 2881,221 | 0,009 | 0,0 |
| P | 7 | 18 | 2882,264 | 0,022 | 0,0 | P | 7 | 17 | 2883,266 | 0,004 | 1,0 |
| P | 7 | 16 | 2884,275 | 0,003 | 1,0 | P | 7 | 15 | 2885,282 | 0,010 | 0,5 |
| P | 7 | 14 | 2886,266 | 0,005 | 0,0 | P | 7 | 13 | 2887,247 | 0,007 | 0,0 |
| P | 7 | 12 | 2888,209 | 0,000 | 0,1 | P | 7 | 11 | 2889,172 | 0,004 | 0,0 |
| P | 7 | 10 | 2890,115 | -0,002 | 0,0 | P | 7 | 9 | 2891,051 | -0,003 | 0,0 |
| P | 7 | 8 | 2891,983 | 0,001 | 0,0 | P | 8 | 35 | 2861,298 | 0,025 | 0,0 |
| P | 8 | 34 | 2862,482 | 0,019 | 0,2 | P | 8 | 33 | 2863,652 | 0,009 | 0,7 |
| P | 8 | 32 | 2864,801 | -0,012 | 0,0 | P | 8 | 31 | 2865,970 | -0,004 | 0,0 |
| P | 8 | 30 | 2867,114 | -0,009 | 0,0 | P | 8 | 29 | 2868,261 | -0,003 | 0,0 |
| P | 8 | 28 | 2869,391 | -0,003 | 0,5 | P | 8 | 27 | 2870,483 | -0,031 | 0,0 |
| P | 8 | 26 | 2871,598 | -0,026 | 0,0 | P | 8 | 25 | 2872,715 | -0,009 | 0,0 |
| P | 8 | 24 | 2873,799 | -0,015 | 0,7 | P | 8 | 23 | 2874,879 | -0,015 | 0,0 |
| P | 8 | 22 | 2875,955 | -0,008 | 0,0 | P | 8 | 21 | 2876,997 | -0,026 | 0,0 |
| P | 8 | 20 | 2878,061 | -0,011 | 0,0 | P | 8 | 19 | 2879,113 | 0,002 | 0,0 |
| P | 8 | 18 | 2880,125 | -0,015 | 0,1 | P | 8 | 17 | 2881,150 | -0,010 | 0,3 |
| P | 8 | 16 | 2882,150 | -0,018 | 0,0 | P | 8 | 15 | 2883,137 | -0,031 | 0,3 |
| P | 8 | 14 | 2884,151 | -0,005 | 0,0 | P | 8 | 13 | 2885,165 | 0,030 | 0,0 |
| P | 8 | 12 | 2886,126 | 0,023 | 0,0 | P | 8 | 11 | 2887,093 | 0,031 | 0,0 |
| P | 8 | 10 | 2888,058 | 0,049 | 0,0 | P | 8 | 9 | 2888,994 | 0,046 | 0,0 |
| Q | 1 | 6 | 2905,211 | -0,005 | 0,1 | Q | 1 | 5 | 2906,118 | -0,006 | 0,1 |
| Q | 1 | 4 | 2905,597 | 0,007 | 0,0 | Q | 1 | 3 | 2906,009 | 0,001 | 0,5 |
| Q | 1 | 2 | 2905,822 | -0,007 | 0,1 | Q | 1 | 1 | 2905,950 | 0,006 | 0,5 |
| Q | 2 | 11 | 2904,836 | -0,009 | 0,0 | Q | 2 | 10 | 2904,896 | 0,002 | 0,1 |
| Q | 2 | 9 | 2905,048 | 0,003 | 0,1 | Q | 2 | 8 | 2905,110 | 0,000 | 0,1 |
| Q | 2 | 7 | 2905,211 | -0,001 | 0,1 | Q | 2 | 6 | 2905,269 | -0,006 | 0,0 |
| Q | 2 | 5 | 2905,355 | 0,011 | 0,1 | Q | 2 | 4 | 2905,396 | 0,002 | 0,0 |
| Q | 2 | 3 | 2905,455 | 0,018 | 0,0 | Q | 2 | 2 | 2905,455 | -0,014 | 0,0 |
| Q | 3 | 13 | 2903,823 | -0,004 | 0,7 | Q | 3 | 12 | 2903,958 | -0,004 | 0,1 |
| Q | 3 | 11 | 2904,098 | 0,009 | 0,2 | Q | 3 | 10 | 2904,217 | 0,013 | 0,0 |
| Q | 3 | 9 | 2904,297 | -0,012 | 0,5 | Q | 3 | 8 | 2904,382 | -0,021 | 0,0 |
| Q | 3 | 7 | 2904,485 | -0,003 | 0,5 | Q | 3 | 6 | 2904,555 | -0,006 | 0,5 |
| Q | 3 | 5 | 2904,628 | 0,004 | 0,0 | Q | 3 | 4 | 2904,667 | -0,009 | 0,0 |
| Q | 3 | 3 | 2904,718 | -0,001 | 0,0 | Q | 4 | 16 | 2902,369 | 0,020 | 0,0 |
| Q | 4 | 15 | 2902,518 | 0,001 | 0,1 | Q | 4 | 14 | 2902,682 | 0,008 | 0,0 |
| Q | 4 | 13 | 2902,835 | 0,015 | 0,0 | Q | 4 | 12 | 2902,963 | 0,006 | 0,0 |
| Q | 4 | 11 | 2903,078 | -0,004 | 0,7 | Q | 4 | 10 | 2903,193 | -0,004 | 0,2 |
| Q | 4 | 9 | 2903,309 | 0,007 | 0,5 | Q | 4 | 8 | 2903,401 | 0,005 | 0,0 |
| Q | 4 | 7 | 2903,475 | -0,004 | 0,5 | Q | 4 | 6 | 2903,552 | -0,001 | 0,2 |
| Q | 4 | 5 | 2903,615 | -0,000 | 0,0 | Q | 4 | 4 | 2903,665 | -0,003 | 0,0 |
| Q | 5 | 16 | 2901,058 | 0,001 | 0,2 | Q | 5 | 15 | 2901,223 | -0,001 | 0,0 |
| Q | 5 | 14 | 2901,377 | -0,004 | 0,5 | Q | 5 | 13 | 2901,532 | 0,006 | 0,1 |
| Q | 5 | 12 | 2901,662 | 0,000 | 0,0 | Q | 5 | 11 | 2901,787 | -0,000 | 1,0 |
| Q | 5 | 10 | 2901,903 | 0,001 | 1,0 | Q | 5 | 9 | 2902,013 | 0,007 | 0,0 |
| Q | 5 | 8 | 2902,097 | -0,003 | 0,0 | Q | 5 | 7 | 2902,186 | 0,003 | 0,5 |
| Q | 5 | 6 | 2902,261 | 0,005 | 0,2 | Q | 5 | 5 | 2902,332 | 0,013 | 0,0 |
| Q | 6 | 20 | 2898,734 | 0,019 | 0,0 | Q | 6 | 19 | 2898,934 | 0,012 | 0,1 |
| Q | 6 | 18 | 2899,120 | 0,000 | 0,1 | Q | 6 | 17 | 2899,313 | 0,007 | 0,0 |
| Q | 6 | 16 | 2899,493 | 0,010 | 0,0 | Q | 6 | 15 | 2899,654 | 0,006 | 0,3 |
| Q | 6 | 14 | 2899,825 | 0,021 | 0,0 | Q | 6 | 13 | 2899,953 | 0,004 | 0,7 |
| Q | 6 | 12 | 2900,090 | 0,006 | 0,0 | Q | 6 | 11 | 2900,226 | 0,018 | 0,0 |
| Q | 6 | 10 | 2900,325 | 0,003 | 0,0 | Q | 6 | 9 | 2900,425 | -0,001 | 0,0 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Q | 6 | 8 | 2900,526 | 0,006 | 0,0 | Q | 6 | 7 | 2900,642 | 0,040 | 0,0 |
| Q | 6 | 6 | 2900,682 | 0,007 | 0,0 | Q | 7 | 16 | 2897,644 | 0,009 | 0,0 |
| Q | 7 | 15 | 2897,795 | -0,005 | 0,1 | Q | 7 | 14 | 2897,963 | 0,008 | 0,3 |
| Q | 7 | 13 | 2898,113 | 0,014 | 0,1 | Q | 7 | 12 | 2898,246 | 0,013 | 0,1 |
| Q | 7 | 11 | 2898,359 | 0,003 | 0,0 | Q | 7 | 10 | 2898,500 | 0,030 | 0,0 |
| Q | 7 | 9 | 2898,577 | 0,004 | 0,0 | Q | 7 | 8 | 2898,658 | -0,008 | 0,0 |
| Q | 7 | 7 | 2898,791 | 0,043 | 0,0 | Q | 8 | 16 | 2895,518 | -0,019 | 0,0 |
| Q | 8 | 15 | 2895,696 | -0,005 | 0,1 | Q | 8 | 14 | 2895,857 | 0,002 | 0,0 |
| Q | 8 | 13 | 2895,973 | -0,025 | 0,0 | Q | 8 | 12 | 2896,118 | -0,014 | 0,0 |
| Q | 8 | 11 | 2896,238 | -0,016 | 0,0 | Q | 8 | 10 | 2896,373 | 0,006 | 0,0 |
| Q | 8 | 9 | 2896,441 | -0,028 | 0,0 | Q | 8 | 8 | 2896,527 | -0,034 | 0,0 |
| R | 0 | 46 | 2932,733 | -0,010 | 0,0 | R | 0 | 44 | 2932,136 | -0,005 | 0,3 |
| R | 0 | 42 | 2931,496 | 0,003 | 0,0 | R | 0 | 40 | 2930,799 | -0,002 | 0,7 |
| R | 0 | 38 | 2930,056 | -0,005 | 0,1 | R | 0 | 36 | 2929,276 | 0,001 | 0,1 |
| R | 0 | 34 | 2928,448 | 0,006 | 0,5 | R | 0 | 32 | 2927,566 | 0,005 | 1,0 |
| R | 0 | 30 | 2926,637 | 0,005 | 0,3 | R | 0 | 28 | 2925,654 | 0,000 | 0,3 |
| R | 0 | 26 | 2924,628 | 0,003 | 1,0 | R | 0 | 24 | 2923,548 | -0,000 | 1,0 |
| R | 0 | 22 | 2922,426 | 0,004 | 0,0 | R | 0 | 20 | 2921,249 | 0,003 | 0,7 |
| R | 0 | 18 | 2920,026 | 0,004 | 0,7 | R | 0 | 16 | 2918,752 | 0,003 | 1,0 |
| R | 0 | 14 | 2917,439 | 0,011 | 0,0 | R | 0 | 12 | 2916,071 | 0,010 | 0,0 |
| R | 0 | 10 | 2914,652 | 0,005 | 0,1 | R | 0 | 8 | 2913,178 | -0,010 | 0,0 |
| R | 0 | 6 | 2911,671 | -0,012 | 0,0 | R | 0 | 4 | 2910,134 | -0,001 | 1,0 |
| R | 0 | 2 | 2908,550 | 0,007 | 0,3 | R | 0 | 0 | 2906,896 | -0,012 | 0,5 |
| R | 1 | 47 | 2932,817 | -0,030 | 0,0 | R | 1 | 46 | 2933,884 | 0,034 | 0,0 |
| R | 1 | 45 | 2932,235 | -0,013 | 0,2 | R | 1 | 44 | 2933,196 | 0,005 | 0,1 |
| R | 1 | 43 | 2931,587 | -0,015 | 0,7 | R | 1 | 42 | 2932,482 | 0,001 | 0,7 |
| R | 1 | 41 | 2930,910 | -0,001 | 0,2 | R | 1 | 40 | 2931,719 | -0,003 | 0,7 |
| R | 1 | 39 | 2930,171 | -0,003 | 0,3 | R | 1 | 38 | 2930,910 | -0,001 | 0,2 |
| R | 1 | 37 | 2929,396 | 0,006 | 0,1 | R | 1 | 36 | 2930,056 | 0,005 | 0,1 |
| R | 1 | 35 | 2928,563 | 0,001 | 0,3 | R | 1 | 34 | 2929,144 | 0,001 | 1,0 |
| R | 1 | 33 | 2927,720 | 0,032 | 0,0 | R | 1 | 32 | 2928,183 | -0,003 | 0,0 |
| R | 1 | 31 | 2926,774 | 0,006 | 0,0 | R | 1 | 30 | 2927,196 | 0,013 | 0,0 |
| R | 1 | 29 | 2925,840 | 0,037 | 0,0 | R | 1 | 28 | 2926,136 | 0,004 | 1,0 |
| R | 1 | 27 | 2924,787 | -0,004 | 0,0 | R | 1 | 26 | 2925,038 | 0,002 | 1,0 |
| R | 1 | 25 | 2923,718 | -0,016 | 0,0 | R | 1 | 24 | 2923,900 | 0,007 | 0,5 |
| R | 1 | 23 | 2922,629 | -0,003 | 0,1 | R | 1 | 22 | 2922,705 | -0,001 | 1,0 |
| R | 1 | 21 | 2921,498 | 0,013 | 0,1 | R | 1 | 20 | 2921,470 | -0,004 | 0,1 |
| R | 1 | 19 | 2920,309 | 0,016 | 0,0 | R | 1 | 18 | 2920,189 | -0,008 | 0,0 |
| R | 1 | 17 | 2919,058 | 0,002 | 0,0 | R | 1 | 16 | 2918,875 | -0,003 | 0,0 |
| R | 1 | 15 | 2917,786 | 0,013 | 0,0 | R | 1 | 14 | 2917,509 | -0,004 | 0,0 |
| R | 1 | 13 | 2916,450 | 0,003 | 1,0 | R | 1 | 12 | 2916,106 | -0,001 | 0,0 |
| R | 1 | 11 | 2915,072 | -0,004 | 0,3 | R | 1 | 10 | 2914,652 | -0,005 | 0,1 |
| R | 1 | 9 | 2913,667 | 0,006 | 0,5 | R | 1 | 8 | 2913,178 | 0,013 | 0,0 |
| R | 1 | 7 | 2912,202 | -0,000 | 1,0 | R | 1 | 6 | 2911,644 | 0,014 | 0,0 |
| R | 1 | 5 | 2910,699 | -0,000 | 1,0 | R | 1 | 4 | 2910,057 | 0,002 | 1,0 |
| R | 1 | 3 | 2909,152 | -0,001 | 1,0 | R | 1 | 2 | 2908,431 | -0,005 | 1,0 |
| R | 1 | 1 | 2907,573 | 0,009 | 0,0 | R | 2 | 47 | 2933,238 | -0,001 | 0,0 |
| R | 2 | 46 | 2933,913 | 0,019 | 0,0 | R | 2 | 45 | 2932,602 | 0,001 | 0,1 |
| R | 2 | 44 | 2933,138 | -0,009 | 0,0 | R | 2 | 43 | 2931,922 | 0,005 | 0,7 |
| R | 2 | 42 | 2932,347 | -0,008 | 0,7 | R | 2 | 41 | 2931,202 | 0,015 | 0,5 |
| R | 2 | 40 | 2931,496 | -0,021 | 0,0 | R | 2 | 39 | 2930,424 | 0,014 | 0,0 |
| R | 2 | 38 | 2930,627 | -0,009 | 0,0 | R | 2 | 37 | 2929,591 | 0,003 | 0,0 |
| R | 2 | 36 | 2929,709 | -0,003 | 1,0 | R | 2 | 35 | 2928,719 | -0,000 | 0,0 |
| R | 2 | 34 | 2928,719 | -0,027 | 0,0 | R | 2 | 33 | 2927,794 | -0,011 | 0,0 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| R | 2 | 32 | 2927,748 | 0,009 | 0,0 | R | 2 | 31 | 2926,841 | -0,005 | 0,0 |
| R | 2 | 30 | 2926,692 | 0,001 | 0,3 | R | 2 | 29 | 2925,840 | -0,002 | 0,0 |
| R | 2 | 28 | 2925,606 | 0,001 | 0,1 | R | 2 | 27 | 2924,787 | -0,005 | 0,0 |
| R | 2 | 26 | 2924,473 | -0,006 | 0,3 | R | 2 | 25 | 2923,718 | 0,020 | 0,0 |
| R | 2 | 24 | 2923,315 | -0,001 | 1,0 | R | 2 | 23 | 2922,562 | 0,002 | 0,5 |
| R | 2 | 22 | 2922,112 | -0,002 | 0,0 | R | 2 | 21 | 2921,383 | 0,007 | 0,0 |
| R | 2 | 20 | 2920,892 | 0,017 | 0,0 | R | 2 | 19 | 2920,155 | 0,005 | 0,0 |
| R | 2 | 18 | 2919,604 | 0,006 | 0,0 | R | 2 | 17 | 2918,875 | -0,004 | 0,0 |
| R | 2 | 16 | 2918,278 | -0,004 | 1,0 | R | 2 | 15 | 2917,532 | -0,033 | 0,0 |
| R | 2 | 14 | 2916,926 | -0,002 | 1,0 | R | 2 | 13 | 2916,201 | -0,006 | 0,2 |
| R | 2 | 12 | 2915,528 | -0,007 | 0,1 | R | 2 | 11 | 2914,802 | -0,004 | 0,0 |
| R | 2 | 10 | 2914,099 | -0,004 | 0,0 | R | 2 | 9 | 2913,367 | 0,006 | 0,0 |
| R | 2 | 8 | 2912,637 | 0,006 | 0,0 | R | 2 | 7 | 2911,882 | 0,008 | 0,0 |
| R | 2 | 6 | 2911,134 | 0,016 | 0,0 | R | 2 | 5 | 2910,368 | 0,023 | 0,0 |
| R | 2 | 4 | 2909,577 | 0,012 | 0,0 | R | 2 | 3 | 2908,774 | 0,002 | 0,1 |
| R | 2 | 2 | 2907,971 | 0,001 | 0,1 | R | 3 | 47 | 2932,905 | 0,001 | 0,1 |
| R | 3 | 46 | 2932,786 | -0,013 | 0,0 | R | 3 | 45 | 2932,235 | 0,009 | 0,1 |
| R | 3 | 44 | 2932,047 | -0,008 | 0,7 | R | 3 | 43 | 2931,496 | -0,008 | 0,0 |
| R | 3 | 42 | 2931,269 | -0,006 | 0,1 | R | 3 | 41 | 2930,731 | -0,007 | 0,1 |
| R | 3 | 40 | 2930,460 | 0,005 | 0,0 | R | 3 | 39 | 2929,930 | 0,001 | 0,5 |
| R | 3 | 37 | 2929,070 | -0,005 | 0,7 | R | 3 | 36 | 2928,719 | 0,018 | 0,0 |
| R | 3 | 35 | 2928,183 | 0,005 | 0,0 | R | 3 | 34 | 2927,789 | 0,023 | 0,0 |
| R | 3 | 33 | 2927,230 | -0,009 | 0,0 | R | 3 | 32 | 2926,774 | -0,017 | 0,0 |
| R | 3 | 31 | 2926,264 | 0,008 | 0,0 | R | 3 | 30 | 2925,791 | 0,015 | 0,0 |
| R | 3 | 29 | 2925,229 | -0,001 | 0,7 | R | 3 | 28 | 2924,719 | -0,002 | 0,5 |
| R | 3 | 27 | 2924,160 | -0,002 | 1,0 | R | 3 | 26 | 2923,621 | -0,005 | 1,0 |
| R | 3 | 25 | 2923,051 | -0,000 | 1,0 | R | 3 | 24 | 2922,484 | -0,005 | 0,2 |
| R | 3 | 23 | 2921,891 | -0,008 | 0,0 | R | 3 | 22 | 2921,319 | 0,007 | 0,0 |
| R | 3 | 21 | 2920,702 | -0,002 | 0,5 | R | 3 | 20 | 2920,095 | 0,001 | 0,0 |
| R | 3 | 19 | 2919,465 | -0,002 | 1,0 | R | 3 | 18 | 2918,837 | 0,003 | 0,0 |
| R | 3 | 17 | 2918,180 | -0,007 | 1,0 | R | 3 | 16 | 2917,532 | -0,001 | 0,0 |
| R | 3 | 15 | 2916,863 | -0,002 | 0,0 | R | 3 | 14 | 2916,201 | 0,011 | 0,0 |
| R | 3 | 13 | 2915,503 | 0,001 | 0,1 | R | 3 | 12 | 2914,802 | -0,003 | 0,1 |
| R | 3 | 11 | 2914,099 | 0,003 | 0,0 | R | 3 | 10 | 2913,367 | -0,011 | 0,0 |
| R | 3 | 9 | 2912,637 | -0,012 | 0,0 | R | 3 | 8 | 2911,882 | -0,027 | 0,0 |
| R | 3 | 7 | 2911,134 | -0,025 | 0,0 | R | 3 | 6 | 2910,400 | 0,001 | 0,0 |
| R | 3 | 5 | 2909,618 | -0,010 | 0,0 | R | 3 | 4 | 2908,849 | 0,003 | 0,0 |
| R | 3 | 3 | 2908,050 | -0,005 | 0,0 | R | 4 | 47 | 2932,050 | 0,081 | 0,0 |
| R | 4 | 46 | 2931,719 | 0,073 | 0,0 | R | 4 | 45 | 2931,335 | 0,056 | 0,1 |
| R | 4 | 44 | 2930,982 | 0,051 | 0,5 | R | 4 | 43 | 2930,624 | 0,078 | 0,0 |
| R | 4 | 42 | 2930,216 | 0,043 | 0,0 | R | 4 | 41 | 2929,818 | 0,046 | 0,5 |
| R | 4 | 40 | 2929,428 | 0,053 | 0,0 | R | 4 | 39 | 2929,000 | 0,045 | 0,7 |
| R | 4 | 38 | 2928,563 | 0,027 | 0,0 | R | 4 | 37 | 2928,133 | 0,037 | 0,0 |
| R | 4 | 36 | 2927,686 | 0,032 | 0,0 | R | 4 | 35 | 2927,230 | 0,035 | 0,0 |
| R | 4 | 34 | 2926,774 | 0,044 | 0,0 | R | 4 | 33 | 2926,264 | 0,013 | 0,1 |
| R | 4 | 32 | 2925,791 | 0,027 | 0,0 | R | 4 | 31 | 2925,287 | 0,022 | 0,2 |
| R | 4 | 30 | 2924,787 | 0,030 | 0,0 | R | 4 | 29 | 2924,252 | 0,014 | 1,0 |
| R | 4 | 28 | 2923,718 | 0,010 | 0,0 | R | 4 | 27 | 2923,183 | 0,016 | 1,0 |
| R | 4 | 26 | 2922,629 | 0,012 | 0,0 | R | 4 | 25 | 2922,074 | 0,018 | 0,0 |
| R | 4 | 24 | 2921,486 | 0,002 | 0,0 | R | 4 | 23 | 2920,892 | -0,009 | 0,0 |
| R | 4 | 22 | 2920,309 | 0,000 | 0,0 | R | 4 | 21 | 2919,709 | 0,004 | 0,7 |
| R | 4 | 20 | 2919,084 | -0,007 | 0,0 | R | 4 | 19 | 2918,476 | 0,009 | 0,5 |
| R | 4 | 18 | 2917,816 | -0,016 | 0,0 | R | 4 | 17 | 2917,185 | -0,001 | 0,0 |
| R | 4 | 16 | 2916,537 | 0,007 | 0,0 | R | 4 | 15 | 2915,883 | 0,019 | 0,0 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| R | 4 | 14 | 2915,195 | 0,008 | 0,0 | R | 4 | 13 | 2914,504 | 0,005 | 0,5 |
| R | 4 | 12 | 2913,795 | -0,007 | 0,5 | R | 4 | 11 | 2913,102 | 0,009 | 0,0 |
| R | 4 | 10 | 2912,365 | -0,009 | 0,0 | R | 4 | 9 | 2911,642 | -0,003 | 0,0 |
| R | 4 | 8 | 2910,903 | -0,001 | 0,0 | R | 4 | 7 | 2910,169 | 0,014 | 0,0 |
| R | 4 | 6 | 2909,389 | -0,005 | 0,2 | R | 4 | 5 | 2908,621 | -0,001 | 0,0 |
| R | 4 | 4 | 2907,841 | 0,001 | 0,1 | R | 5 | 42 | 2928,851 | -0,049 | 0,0 |
| R | 5 | 41 | 2928,448 | -0,057 | 0,0 | R | 5 | 40 | 2928,073 | -0,029 | 0,0 |
| R | 5 | 39 | 2927,686 | -0,001 | 0,0 | R | 5 | 38 | 2927,230 | -0,033 | 0,0 |
| R | 5 | 37 | 2926,808 | -0,018 | 0,0 | R | 5 | 36 | 2926,349 | -0,032 | 1,0 |
| R | 5 | 35 | 2925,894 | -0,029 | 0,0 | R | 5 | 34 | 2925,435 | -0,021 | 0,7 |
| R | 5 | 33 | 2924,958 | -0,020 | 1,0 | R | 5 | 32 | 2924,473 | -0,017 | 0,0 |
| R | 5 | 31 | 2923,968 | -0,023 | 0,5 | R | 5 | 30 | 2923,457 | -0,025 | 0,1 |
| R | 5 | 29 | 2922,946 | -0,015 | 0,5 | R | 5 | 28 | 2922,426 | -0,005 | 0,0 |
| R | 5 | 27 | 2921,891 | 0,001 | 0,0 | R | 5 | 26 | 2921,319 | -0,019 | 0,0 |
| R | 5 | 25 | 2920,766 | -0,011 | 1,0 | R | 5 | 24 | 2920,189 | -0,014 | 0,0 |
| R | 5 | 23 | 2919,604 | -0,016 | 0,0 | R | 5 | 22 | 2919,058 | 0,031 | 0,0 |
| R | 5 | 21 | 2918,422 | 0,000 | 0,5 | R | 5 | 20 | 2917,816 | 0,008 | 0,0 |
| R | 5 | 19 | 2917,185 | 0,003 | 0,0 | R | 5 | 18 | 2916,537 | -0,009 | 0,0 |
| R | 5 | 17 | 2915,883 | -0,017 | 0,0 | R | 5 | 16 | 2915,237 | -0,006 | 0,0 |
| R | 5 | 15 | 2914,574 | -0,002 | 0,7 | R | 5 | 14 | 2913,891 | -0,007 | 0,7 |
| R | 5 | 13 | 2913,178 | -0,032 | 0,0 | R | 5 | 12 | 2912,504 | -0,007 | 0,3 |
| R | 5 | 11 | 2911,812 | 0,010 | 0,0 | R | 5 | 10 | 2911,065 | -0,017 | 0,0 |
| R | 5 | 9 | 2910,367 | 0,015 | 0,0 | R | 5 | 8 | 2909,618 | 0,007 | 0,0 |
| R | 5 | 7 | 2908,851 | -0,009 | 0,0 | R | 5 | 6 | 2908,096 | -0,003 | 0,0 |
| R | 5 | 5 | 2907,318 | -0,008 | 0,0 | R | 6 | 42 | 2927,362 | -0,006 | 0,0 |
| R | 6 | 41 | 2926,977 | 0,004 | 0,3 | R | 6 | 40 | 2926,566 | -0,001 | 0,3 |
| R | 6 | 39 | 2926,136 | -0,015 | 0,0 | R | 6 | 38 | 2925,723 | -0,002 | 0,0 |
| R | 6 | 37 | 2925,287 | -0,000 | 0,0 | R | 6 | 36 | 2924,843 | 0,004 | 0,0 |
| R | 6 | 35 | 2924,379 | -0,002 | 0,7 | R | 6 | 34 | 2923,900 | -0,012 | 0,0 |
| R | 6 | 33 | 2923,417 | -0,016 | 0,0 | R | 6 | 32 | 2922,946 | 0,003 | 0,1 |
| R | 6 | 31 | 2922,426 | -0,016 | 0,0 | R | 6 | 30 | 2921,891 | -0,040 | 0,0 |
| R | 6 | 29 | 2921,383 | -0,026 | 0,0 | R | 6 | 28 | 2920,892 | 0,015 | 0,0 |
| R | 6 | 27 | 2920,309 | -0,026 | 0,0 | R | 6 | 26 | 2919,783 | 0,001 | 0,7 |
| R | 6 | 25 | 2919,225 | 0,006 | 0,5 | R | 6 | 24 | 2918,651 | 0,007 | 0,5 |
| R | 6 | 23 | 2918,064 | 0,004 | 0,7 | R | 6 | 22 | 2917,487 | 0,022 | 0,0 |
| R | 6 | 21 | 2916,863 | 0,004 | 0,0 | R | 6 | 20 | 2916,255 | 0,012 | 0,0 |
| R | 6 | 19 | 2915,625 | 0,009 | 0,1 | R | 6 | 18 | 2915,002 | 0,022 | 0,1 |
| R | 6 | 17 | 2914,338 | 0,006 | 0,2 | R | 6 | 16 | 2913,708 | 0,034 | 0,0 |
| R | 6 | 15 | 2913,016 | 0,011 | 0,0 | R | 6 | 14 | 2912,339 | 0,012 | 0,0 |
| R | 6 | 13 | 2911,642 | 0,004 | 0,0 | R | 6 | 12 | 2910,950 | 0,012 | 0,0 |
| R | 6 | 11 | 2910,230 | 0,003 | 0,0 | R | 6 | 10 | 2909,528 | 0,021 | 0,0 |
| R | 6 | 9 | 2908,779 | 0,004 | 0,0 | R | 6 | 8 | 2908,050 | 0,016 | 0,0 |
| R | 6 | 7 | 2907,295 | 0,012 | 0,0 | R | 6 | 6 | 2906,538 | 0,018 | 0,0 |

# FREQUENCIES FOR THE (2,0,1) BAND OF $^{14}NO_2$

| | K | N | OBS | O-C | WT | | K | N | OBS | O-C | WT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| P | 0 | 48 | 4121.895 | 0.004 | 0.3 | P | 0 | 46 | 4125.050 | 0.002 | 0.3 |
| P | 0 | 44 | 4128.131 | -0.008 | 1.0 | P | 0 | 42 | 4131.140 | -0.023 | 0.0 |
| P | 0 | 40 | 4134.113 | -0.009 | 1.0 | P | 0 | 38 | 4137.003 | -0.011 | 0.1 |
| P | 0 | 36 | 4139.829 | -0.012 | 1.0 | P | 0 | 34 | 4142.596 | -0.006 | 0.1 |
| P | 0 | 32 | 4145.290 | -0.009 | 0.5 | P | 0 | 30 | 4147.920 | -0.010 | 1.0 |
| P | 0 | 18 | 4162.393 | -0.000 | 0.7 | P | 0 | 16 | 4164.583 | -0.004 | 1.0 |
| P | 0 | 14 | 4166.719 | -0.001 | 1.0 | P | 0 | 12 | 4168.789 | -0.003 | 1.0 |
| P | 0 | 10 | 4170.800 | -0.002 | 1.0 | P | 0 | 8 | 4172.752 | 0.000 | 0.5 |
| P | 0 | 6 | 4174.645 | 0.004 | 0.7 | P | 1 | 48 | 4121.747 | -0.003 | 0.0 |
| P | 1 | 47 | 4123.464 | 0.009 | 1.0 | P | 1 | 46 | 4124.875 | -0.002 | 0.7 |
| P | 1 | 45 | 4126.586 | 0.005 | 1.0 | P | 1 | 44 | 4127.937 | -0.004 | 1.0 |
| P | 1 | 43 | 4129.643 | 0.002 | 1.0 | P | 1 | 42 | 4130.936 | -0.005 | 0.7 |
| P | 1 | 41 | 4132.637 | -0.001 | 1.0 | P | 1 | 40 | 4133.874 | -0.004 | 1.0 |
| P | 1 | 39 | 4135.563 | -0.005 | 0.7 | P | 1 | 38 | 4136.749 | -0.005 | 1.0 |
| P | 1 | 37 | 4138.432 | -0.001 | 1.0 | P | 1 | 36 | 4139.562 | -0.006 | 1.0 |
| P | 1 | 35 | 4141.231 | -0.002 | 0.3 | P | 1 | 34 | 4142.314 | -0.006 | 1.0 |
| P | 1 | 32 | 4145.007 | -0.004 | 1.0 | P | 1 | 31 | 4146.637 | -0.003 | 0.7 |
| P | 1 | 30 | 4147.638 | -0.004 | 1.0 | P | 1 | 28 | 4150.204 | -0.007 | 1.0 |
| P | 1 | 23 | 4156.676 | -0.008 | 0.5 | P | 1 | 21 | 4159.031 | -0.004 | 1.0 |
| P | 1 | 20 | 4159.885 | -0.003 | 1.0 | P | 1 | 19 | 4161.319 | -0.003 | 1.0 |
| P | 1 | 18 | 4162.154 | -0.002 | 1.0 | P | 1 | 17 | 4163.543 | -0.002 | 0.7 |
| P | 1 | 16 | 4164.364 | -0.001 | 1.0 | P | 1 | 15 | 4165.702 | -0.002 | 1.0 |
| P | 1 | 14 | 4166.514 | 0.000 | 0.7 | P | 1 | 13 | 4167.799 | -0.001 | 1.0 |
| P | 1 | 12 | 4168.607 | 0.004 | 0.1 | P | 1 | 11 | 4169.832 | -0.000 | 0.7 |
| P | 1 | 8 | 4172.601 | 0.002 | 0.0 | P | 1 | 4 | 4176.361 | 0.005 | 1.0 |
| P | 1 | 3 | 4177.315 | -0.009 | 0.1 | P | 1 | 2 | 4178.142 | -0.001 | 0.2 |
| P | 2 | 48 | 4121.597 | 0.016 | 0.3 | P | 2 | 47 | 4123.208 | 0.040 | 0.2 |
| P | 2 | 46 | 4124.711 | 0.014 | 0.5 | P | 2 | 44 | 4127.766 | 0.012 | 0.7 |
| P | 2 | 42 | 4130.764 | 0.013 | 0.5 | P | 2 | 41 | 4132.329 | 0.027 | 0.1 |
| P | 2 | 39 | 4135.235 | 0.015 | 0.7 | P | 2 | 38 | 4136.575 | 0.007 | 0.0 |
| P | 2 | 37 | 4138.086 | 0.010 | 1.0 | P | 2 | 35 | 4140.878 | 0.010 | 1.0 |
| P | 2 | 34 | 4142.152 | 0.005 | 0.7 | P | 2 | 33 | 4143.606 | 0.008 | 1.0 |
| P | 2 | 32 | 4144.852 | 0.005 | 1.0 | P | 2 | 31 | 4146.273 | 0.008 | 1.0 |
| P | 2 | 30 | 4147.493 | 0.004 | 1.0 | P | 2 | 29 | 4148.874 | 0.004 | 1.0 |
| P | 2 | 28 | 4150.072 | 0.003 | 1.0 | P | 2 | 27 | 4151.416 | 0.004 | 1.0 |
| P | 2 | 26 | 4152.593 | 0.004 | 1.0 | P | 2 | 25 | 4153.895 | 0.003 | 1.0 |
| P | 2 | 24 | 4155.049 | 0.001 | 1.0 | P | 2 | 23 | 4156.311 | -0.000 | 0.0 |
| P | 2 | 19 | 4160.960 | -0.002 | 0.7 | P | 2 | 18 | 4162.051 | -0.001 | 1.0 |
| P | 2 | 17 | 4163.196 | 0.002 | 1.0 | P | 2 | 16 | 4164.262 | 0.001 | 1.0 |
| P | 2 | 15 | 4165.365 | 0.001 | 1.0 | P | 2 | 14 | 4166.413 | 0.004 | 0.7 |
| P | 2 | 13 | 4167.476 | 0.003 | 1.0 | P | 2 | 12 | 4168.494 | 0.002 | 1.0 |
| P | 2 | 11 | 4169.518 | -0.001 | 1.0 | P | 2 | 10 | 4170.510 | -0.002 | 0.3 |
| P | 2 | 9 | 4171.506 | 0.002 | 0.2 | P | 2 | 8 | 4172.469 | 0.001 | 0.5 |
| P | 2 | 6 | 4174.362 | 0.000 | 0.0 | P | 2 | 4 | 4176.198 | 0.006 | 0.7 |
| P | 3 | 48 | 4121.339 | 0.111 | 0.0 | P | 3 | 47 | 4122.921 | 0.125 | 0.0 |
| P | 3 | 46 | 4124.453 | 0.099 | 0.0 | P | 3 | 45 | 4126.006 | 0.108 | 0.0 |
| P | 3 | 44 | 4127.512 | 0.091 | 0.0 | P | 3 | 43 | 4129.029 | 0.090 | 0.0 |
| P | 3 | 42 | 4130.507 | 0.080 | 0.0 | P | 3 | 39 | 4134.900 | 0.068 | 0.0 |
| P | 3 | 38 | 4136.321 | 0.063 | 0.0 | P | 3 | 37 | 4137.748 | 0.061 | 0.0 |
| P | 3 | 34 | 4141.893 | 0.048 | 0.0 | P | 3 | 33 | 4143.257 | 0.046 | 0.0 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| P | 3 | 32 | 4144,587 | 0,041 | 0.0 | P | 3 | 31 | 4145,920 | 0,039 | 0.0 |
| P | 3 | 30 | 4147,221 | 0,035 | 0.0 | P | 3 | 29 | 4148,520 | 0,032 | 0.0 |
| P | 3 | 28 | 4149,794 | 0,030 | 0.0 | P | 3 | 27 | 4151,059 | 0,025 | 0.0 |
| P | 3 | 26 | 4152,302 | 0,022 | 0.0 | P | 3 | 25 | 4153,542 | 0,025 | 0.0 |
| P | 3 | 19 | 4160,606 | 0,009 | 0.0 | P | 3 | 18 | 4161,728 | 0,007 | 0.0 |
| P | 3 | 17 | 4162,840 | 0,008 | 0.0 | P | 3 | 16 | 4163,931 | 0,005 | 0.0 |
| P | 3 | 15 | 4165,011 | 0,006 | 0.0 | P | 3 | 10 | 4170,163 | -0,003 | 0.1 |
| P | 3 | 9 | 4171,152 | 0,001 | 0.5 | P | 3 | 8 | 4172,122 | 0,002 | 0.7 |
| P | 3 | 7 | 4173,076 | 0,001 | 0.5 | P | 3 | 6 | 4174,019 | 0,006 | 0.1 |
| P | 3 | 5 | 4174,927 | -0,008 | 0.5 | P | 3 | 4 | 4175,840 | -0,002 | 0.0 |
| P | 4 | 48 | 4120,646 | -0,077 | 0.1 | P | 4 | 47 | 4122,231 | -0,065 | 0.1 |
| P | 4 | 46 | 4123,796 | -0,058 | 0.1 | P | 4 | 45 | 4125,348 | -0,049 | 0.7 |
| P | 4 | 44 | 4126,880 | -0,044 | 0.5 | P | 4 | 43 | 4128,401 | -0,036 | 0.2 |
| P | 4 | 42 | 4129,905 | -0,028 | 0.7 | P | 4 | 41 | 4131,384 | -0,030 | 1.0 |
| P | 4 | 40 | 4132,860 | -0,020 | 1.0 | P | 4 | 39 | 4134,315 | -0,016 | 1.0 |
| P | 4 | 35 | 4139,969 | -0,010 | 0.5 | P | 4 | 34 | 4141,345 | -0,007 | 1.0 |
| P | 4 | 33 | 4142,705 | -0,005 | 1.0 | P | 4 | 32 | 4144,047 | -0,005 | 1.0 |
| P | 4 | 31 | 4145,375 | -0,004 | 1.0 | P | 4 | 30 | 4146,687 | -0,003 | 1.0 |
| P | 4 | 29 | 4147,984 | -0,003 | 1.0 | P | 4 | 22 | 4156,627 | 0,001 | 0.5 |
| P | 4 | 20 | 4158,953 | -0,001 | 1.0 | P | 4 | 18 | 4161,220 | -0,001 | 1.0 |
| P | 4 | 17 | 4162,334 | 0,004 | 0.7 | P | 4 | 16 | 4163,420 | -0,005 | 1.0 |
| P | 4 | 15 | 4164,503 | -0,001 | 1.0 | P | 4 | 14 | 4165,564 | -0,003 | 1.0 |
| P | 4 | 13 | 4166,611 | -0,004 | 1.0 | P | 4 | 12 | 4167,644 | -0,002 | 1.0 |
| P | 4 | 11 | 4168,657 | -0,006 | 0.3 | P | 4 | 10 | 4169,659 | -0,005 | 1.0 |
| P | 4 | 8 | 4171,617 | -0,002 | 0.1 | P | 4 | 6 | 4173,507 | -0,005 | 0.1 |
| P | 5 | 46 | 4123,274 | 0,051 | 0.3 | P | 5 | 45 | 4124,814 | 0,049 | 0.1 |
| P | 5 | 43 | 4127,843 | 0,041 | 0.3 | P | 5 | 41 | 4130,805 | 0,028 | 0.1 |
| P | 5 | 40 | 4132,275 | 0,033 | 0.1 | P | 5 | 38 | 4135,156 | 0,031 | 0.1 |
| P | 5 | 36 | 4137,971 | 0,025 | 0.5 | P | 5 | 34 | 4140,727 | 0,021 | 0.7 |
| P | 5 | 33 | 4142,087 | 0,024 | 0.5 | P | 5 | 32 | 4143,423 | 0,019 | 1.0 |
| P | 5 | 31 | 4144,744 | 0,014 | 1.0 | P | 5 | 30 | 4146,055 | 0,015 | 1.0 |
| P | 5 | 29 | 4147,347 | 0,012 | 1.0 | P | 5 | 28 | 4148,624 | 0,009 | 1.0 |
| P | 5 | 27 | 4149,884 | 0,007 | 1.0 | P | 5 | 26 | 4151,135 | 0,007 | 1.0 |
| P | 5 | 25 | 4152,363 | 0,002 | 1.0 | P | 5 | 18 | 4160,559 | -0,001 | 0.2 |
| P | 5 | 17 | 4161,666 | -0,004 | 1.0 | P | 5 | 16 | 4162,761 | -0,002 | 1.0 |
| P | 5 | 15 | 4163,840 | -0,001 | 1.0 | P | 5 | 14 | 4164,897 | -0,007 | 0.5 |
| P | 5 | 13 | 4165,946 | -0,005 | 1.0 | P | 5 | 12 | 4166,982 | -0,001 | 1.0 |
| P | 5 | 11 | 4167,997 | -0,003 | 0.5 | P | 5 | 10 | 4168,996 | -0,005 | 0.5 |
| P | 5 | 9 | 4169,979 | -0,006 | 0.5 | P | 5 | 8 | 4170,947 | -0,009 | 0.3 |
| P | 5 | 7 | 4171,898 | -0,011 | 0.1 | P | 6 | 47 | 4120,955 | 0,036 | 0.1 |
| P | 6 | 46 | 4122,506 | 0,034 | 0.1 | P | 6 | 45 | 4124,047 | 0,037 | 0.1 |
| P | 6 | 44 | 4125,561 | 0,029 | 0.1 | P | 6 | 43 | 4127,068 | 0,029 | 0.1 |
| P | 6 | 42 | 4128,554 | 0,024 | 0.1 | P | 6 | 41 | 4130,030 | 0,024 | 0.2 |
| P | 6 | 40 | 4131,490 | 0,023 | 0.1 | P | 6 | 39 | 4132,934 | 0,020 | 0.5 |
| P | 6 | 38 | 4134,365 | 0,022 | 0.3 | P | 6 | 34 | 4139,925 | 0,014 | 0.0 |
| P | 6 | 33 | 4141,275 | 0,010 | 0.0 | P | 6 | 29 | 4146,530 | 0,004 | 1.0 |
| P | 6 | 28 | 4147,808 | 0,004 | 1.0 | P | 6 | 27 | 4149,071 | 0,006 | 1.0 |
| P | 6 | 26 | 4150,310 | -0,001 | 1.0 | P | 6 | 25 | 4151,543 | 0,001 | 1.0 |
| P | 6 | 23 | 4153,955 | -0,003 | 0.7 | P | 6 | 19 | 4158,604 | -0,001 | 0.3 |
| P | 6 | 18 | 4159,726 | -0,002 | 0.3 | P | 6 | 17 | 4160,830 | -0,006 | 0.1 |
| P | 6 | 8 | 4170,100 | -0,013 | 0.1 | P | 6 | 7 | 4171,048 | -0,019 | 0.0 |
| P | 7 | 43 | 4126,133 | -0,020 | 0.2 | P | 7 | 42 | 4127,623 | -0,014 | 0.1 |
| P | 7 | 41 | 4129,090 | -0,016 | 0.1 | P | 7 | 37 | 4134,824 | -0,005 | 0.1 |
| P | 7 | 36 | 4136,214 | -0,008 | 0.5 | P | 7 | 35 | 4137,590 | -0,010 | 0.5 |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| P | 7 | 34 | 4138.953 | -0,010 | 0.5 | | P | 7 | 33 | 4140,303 | -0,008 | 0.5 |
| P | 7 | 32 | 4141,634 | -0,010 | 1.0 | | P | 7 | 31 | 4142,954 | -0,007 | 0.7 |
| P | 7 | 30 | 4144,257 | -0,006 | 1.0 | | P | 7 | 28 | 4146,815 | -0,007 | 1.0 |
| P | 7 | 27 | 4148.069 | -0,009 | 1.0 | | P | 7 | 21 | 4155,296 | -0,005 | 0.7 |
| P | 7 | 20 | 4156,448 | -0,004 | 1.0 | | P | 8 | 35 | 4136,481 | -0,018 | 0.1 |
| P | 8 | 34 | 4137,827 | -0,024 | 0.0 | | P | 8 | 31 | 4141,818 | -0,002 | 0.3 |
| P | 8 | 29 | 4144,388 | -0,003 | 1.0 | | P | 8 | 28 | 4145,656 | 0,002 | 1.0 |
| P | 8 | 27 | 4146.908 | 0,005 | 0.5 | | P | 8 | 26 | 4148,143 | 0,006 | 1.0 |
| P | 8 | 25 | 4149,362 | 0,007 | 0.1 | | P | 8 | 20 | 4155,247 | 0,020 | 0.3 |
| P | 8 | 19 | 4156.378 | 0,021 | 0.3 | | Q | 1 | 1 | 4179,881 | 0,003 | 0.1 |
| Q | 1 | 2 | 4179,752 | 0,000 | 1.0 | | Q | 1 | 3 | 4179,915 | -0,003 | 0.0 |
| Q | 1 | 5 | 4179,993 | 0,003 | 0.1 | | Q | 1 | 7 | 4180,097 | 0,002 | 0.0 |
| Q | 1 | 9 | 4180.230 | -0,002 | 0.0 | | Q | 1 | 11 | 4180,397 | -0,002 | 0.0 |
| Q | 2 | 3 | 4179,575 | 0,005 | 0.2 | | Q | 2 | 2 | 4179,616 | -0,000 | 0.2 |
| Q | 2 | 4 | 4179.507 | 0,000 | 0.1 | | Q | 2 | 5 | 4179,433 | 0,002 | 1.0 |
| Q | 2 | 6 | 4179,332 | 0,000 | 1.0 | | Q | 3 | 3 | 4179,222 | 0,002 | 1.0 |
| Q | 3 | 4 | 4179.160 | 0,002 | 1.0 | | Q | 3 | 5 | 4179,083 | 0,004 | 0.7 |
| Q | 3 | 6 | 4178.986 | 0,000 | 1.0 | | Q | 3 | 7 | 4178,877 | 0,000 | 1.0 |
| Q | 3 | 8 | 4178.754 | 0,002 | 1.0 | | Q | 3 | 9 | 4178,615 | 0,004 | 0.0 |
| Q | 3 | 10 | 4178.455 | 0,001 | 0.0 | | Q | 4 | 4 | 4178,654 | -0,004 | 0.0 |
| Q | 4 | 5 | 4178.583 | 0,002 | 0.0 | | Q | 4 | 6 | 4178,479 | -0,007 | 0.0 |
| Q | 4 | 7 | 4178,379 | 0,002 | 1.0 | | Q | 4 | 8 | 4178,243 | -0,009 | 0.0 |
| Q | 4 | 9 | 4178,099 | -0,012 | 0.0 | | Q | 4 | 10 | 4177,949 | -0,007 | 0.0 |
| Q | 4 | 11 | 4177.788 | 0,005 | 0.0 | | Q | 5 | 5 | 4177,913 | -0,006 | 0.0 |
| Q | 5 | 6 | 4177.818 | -0,007 | 0.0 | | Q | 5 | 7 | 4177,709 | -0,007 | 0.1 |
| Q | 5 | 8 | 4177,588 | -0,003 | 1.0 | | Q | 5 | 9 | 4177,443 | -0,007 | 1.0 |
| Q | 5 | 10 | 4177.310 | 0,015 | 0.0 | | Q | 5 | 11 | 4177,120 | -0,004 | 0.3 |
| Q | 5 | 12 | 4176,941 | 0,004 | 0.0 | | Q | 5 | 13 | 4176,740 | 0,006 | 0.0 |
| Q | 5 | 14 | 4176.510 | -0,006 | 0.0 | | Q | 5 | 15 | 4176,289 | 0,007 | 0.0 |
| Q | 5 | 16 | 4176,038 | 0,006 | 0.5 | | Q | 5 | 17 | 4175,767 | -0,000 | 0.0 |
| Q | 5 | 18 | 4175,496 | 0,009 | 0.0 | | Q | 6 | 6 | 4176,978 | -0,007 | 0.0 |
| Q | 6 | 7 | 4176.875 | -0,002 | 0.7 | | Q | 6 | 8 | 4176,740 | -0,012 | 0.0 |
| Q | 6 | 9 | 4176,609 | -0,005 | 0.3 | | Q | 6 | 10 | 4176,467 | 0,009 | 0.0 |
| Q | 6 | 11 | 4176.289 | 0,001 | 0.0 | | Q | 6 | 12 | 4176,104 | 0,002 | 0.2 |
| Q | 6 | 13 | 4175,887 | -0,014 | 0.0 | | Q | 6 | 14 | 4175,686 | 0,002 | 0.0 |
| Q | 6 | 15 | 4175.442 | -0,010 | 0.0 | | Q | 7 | 7 | 4175,887 | 0,050 | 0.0 |
| Q | 7 | 8 | 4175.767 | 0,053 | 0.0 | | Q | 7 | 9 | 4175,584 | 0,008 | 0.0 |
| Q | 7 | 10 | 4175.442 | 0,018 | 0.0 | | Q | 7 | 11 | 4175,276 | 0,020 | 0.0 |
| Q | 7 | 12 | 4175.077 | 0,005 | 0.0 | | Q | 7 | 13 | 4174,888 | 0,015 | 0.0 |
| R | 0 | 46 | 4200.609 | 0,002 | 0.0 | | R | 0 | 44 | 4200,516 | 0,002 | 0.0 |
| R | 0 | 42 | 4200.330 | -0,022 | 0.0 | | R | 0 | 40 | 4200,112 | -0,011 | 0.0 |
| R | 0 | 38 | 4199,813 | -0,009 | 0.0 | | R | 0 | 36 | 4199,452 | -0,080 | 0.0 |
| R | 0 | 34 | 4199.000 | -0,011 | 0.0 | | R | 0 | 32 | 4198,494 | -0,006 | 0.0 |
| R | 0 | 30 | 4197.901 | -0,016 | 0.0 | | R | 0 | 28 | 4197,252 | -0,010 | 0.0 |
| R | 0 | 26 | 4196,522 | -0,013 | 0.0 | | R | 0 | 24 | 4195,717 | -0,020 | 0.1 |
| R | 0 | 22 | 4194.855 | -0,012 | 0.0 | | R | 0 | 20 | 4193,930 | 0,004 | 0.0 |
| R | 0 | 18 | 4192,928 | 0,015 | 0.0 | | R | 0 | 16 | 4191,843 | 0,011 | 0.0 |
| R | 0 | 14 | 4190,697 | 0,016 | 0.0 | | R | 0 | 12 | 4189,470 | 0,008 | 0.0 |
| R | 0 | 10 | 4188.175 | -0,001 | 0.0 | | R | 0 | 8 | 4186,831 | 0,007 | 0.0 |
| R | 0 | 6 | 4185,408 | 0,002 | 0.0 | | R | 0 | 4 | 4183,924 | 0,000 | 0.0 |
| R | 0 | 2 | 4182,369 | -0,008 | 0.0 | | R | 0 | 0 | 4180,769 | 0,002 | 1.0 |
| R | 1 | 47 | 4200.514 | 0,081 | 0.0 | | R | 1 | 46 | 4202,175 | 0,003 | 0.0 |
| R | 1 | 45 | 4200,417 | 0,060 | 0.0 | | R | 1 | 44 | 4201,989 | 0,000 | 0.5 |
| R | 1 | 43 | 4200.284 | 0,075 | 0.0 | | R | 1 | 42 | 4201,731 | -0,000 | 0.1 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| R | 1 | 41 | 4200.058 | 0,064 | 0.0 | R | 1 | 40 | 4201,394 | -0,007 | 0.1 |
| R | 1 | 39 | 4199.758 | 0,049 | 0.0 | R | 1 | 38 | 4200,995 | -0,004 | 0.2 |
| R | 1 | 37 | 4199.357 | 0,002 | 0.0 | R | 1 | 36 | 4200,516 | -0,010 | 0.2 |
| R | 1 | 35 | 4198.929 | -0,005 | 0.0 | R | 1 | 34 | 4199,973 | -0,010 | 0.0 |
| R | 1 | 33 | 4198.449 | 0,006 | 0.0 | R | 1 | 32 | 4199,357 | -0,012 | 0.0 |
| R | 1 | 31 | 4197.901 | 0,016 | 0.0 | R | 1 | 30 | 4198,688 | -0,001 | 0.3 |
| R | 1 | 29 | 4197.252 | -0,007 | 0.0 | R | 1 | 28 | 4197,929 | -0,011 | 0.0 |
| R | 1 | 27 | 4196.554 | -0,011 | 0.0 | R | 1 | 26 | 4197,118 | -0,007 | 0.3 |
| R | 1 | 25 | 4195.808 | 0,005 | 0.0 | R | 1 | 24 | 4196,243 | -0,000 | 0.0 |
| R | 1 | 23 | 4194.969 | -0,006 | 0.1 | R | 1 | 22 | 4195,291 | -0,006 | 0.1 |
| R | 1 | 21 | 4194.078 | -0,001 | 0.3 | R | 1 | 20 | 4194,279 | -0,007 | 0.0 |
| R | 1 | 19 | 4193.114 | -0,002 | 1.0 | R | 1 | 18 | 4193,214 | 0,003 | 0.0 |
| R | 1 | 17 | 4192.086 | -0,001 | 0.5 | R | 1 | 16 | 4192,063 | -0,008 | 0.5 |
| R | 1 | 15 | 4190.990 | -0,001 | 0.0 | R | 1 | 14 | 4190,864 | -0,004 | 1.0 |
| R | 1 | 13 | 4189.836 | 0,007 | 0.0 | R | 1 | 12 | 4189,603 | -0,000 | 0.0 |
| R | 1 | 11 | 4188.599 | -0,003 | 0.0 | R | 1 | 10 | 4188,271 | -0,004 | 0.0 |
| R | 1 | 9 | 4187.309 | -0,001 | 1.0 | R | 1 | 8 | 4186,890 | 0,004 | 0.0 |
| R | 1 | 7 | 4185.948 | -0,003 | 0.1 | R | 1 | 6 | 4185,423 | -0,011 | 0.0 |
| R | 1 | 5 | 4184.527 | -0,001 | 1.0 | R | 1 | 4 | 4183,924 | 0,003 | 0.0 |
| R | 1 | 3 | 4183.042 | 0,003 | 0.5 | R | 1 | 2 | 4182,354 | 0,008 | 0.0 |
| R | 1 | 1 | 4181.491 | 0,004 | 1.0 | R | 2 | 47 | 4201,334 | 0,031 | 0.0 |
| R | 2 | 46 | 4202.459 | 0,011 | 0.7 | R | 2 | 45 | 4201,206 | 0,039 | 0.7 |
| R | 2 | 44 | 4202.175 | 0,015 | 0.1 | R | 2 | 43 | 4200,995 | 0,035 | 0.0 |
| R | 2 | 42 | 4201.813 | 0,006 | 0.5 | R | 2 | 41 | 4200,722 | 0,037 | 0.0 |
| R | 2 | 40 | 4201.394 | 0,006 | 0.1 | R | 2 | 39 | 4200,362 | 0,019 | 0.0 |
| R | 2 | 38 | 4200.916 | 0,010 | 0.0 | R | 2 | 37 | 4199,949 | 0,018 | 0.0 |
| R | 2 | 36 | 4200.362 | 0,001 | 0.0 | R | 2 | 35 | 4199,464 | 0,010 | 0.0 |
| R | 2 | 34 | 4199.758 | 0,002 | 0.0 | R | 2 | 33 | 4198,929 | 0,020 | 0.0 |
| R | 2 | 32 | 4199.103 | 0,013 | 0.0 | R | 2 | 31 | 4198,310 | 0,014 | 1.0 |
| R | 2 | 30 | 4198.374 | 0,010 | 0.1 | R | 2 | 29 | 4197,621 | 0,003 | 0.0 |
| R | 2 | 28 | 4197.587 | 0,007 | 0.0 | R | 2 | 27 | 4196,875 | 0,002 | 0.0 |
| R | 2 | 26 | 4196.740 | 0,001 | 1.0 | R | 2 | 25 | 4196,069 | 0,007 | 0.0 |
| R | 2 | 24 | 4195.842 | 0,002 | 0.0 | R | 2 | 23 | 4195,194 | 0,008 | 1.0 |
| R | 2 | 22 | 4194.874 | -0,009 | 0.0 | R | 2 | 21 | 4194,258 | 0,014 | 0.0 |
| R | 2 | 20 | 4193.873 | 0,004 | 0.0 | R | 2 | 19 | 4193,238 | -0,001 | 0.0 |
| R | 2 | 18 | 4192.798 | -0,000 | 0.3 | R | 2 | 17 | 4192,166 | -0,002 | 1.0 |
| R | 2 | 16 | 4191.672 | 0,003 | 0.7 | R | 2 | 15 | 4191,026 | -0,007 | 0.0 |
| R | 2 | 14 | 4190.483 | 0,002 | 0.0 | R | 2 | 13 | 4189,836 | 0,003 | 0.0 |
| R | 2 | 12 | 4189.242 | 0,006 | 0.5 | R | 2 | 11 | 4188,569 | -0,001 | 0.0 |
| R | 2 | 10 | 4187.931 | 0,001 | 1.0 | R | 2 | 9 | 4187,248 | 0,004 | 0.7 |
| R | 2 | 8 | 4186.566 | 0,001 | 0.7 | R | 2 | 7 | 4185,855 | 0,001 | 0.5 |
| R | 2 | 6 | 4185.142 | 0,003 | 0.1 | R | 2 | 5 | 4184,399 | -0,001 | 0.3 |
| R | 2 | 4 | 4183.654 | 0,003 | 0.0 | R | 2 | 3 | 4182,886 | 0,002 | 0.0 |
| R | 2 | 2 | 4182.107 | 0,005 | 0.7 | R | 3 | 47 | 4201,532 | 0,149 | 0.0 |
| R | 3 | 46 | 4201.683 | 0,112 | 0.0 | R | 3 | 45 | 4201,335 | 0,138 | 0.0 |
| R | 3 | 44 | 4201.394 | 0,095 | 0.0 | R | 3 | 43 | 4201,054 | 0,109 | 0.0 |
| R | 3 | 42 | 4201.054 | 0,084 | 0.0 | R | 3 | 41 | 4200,722 | 0,094 | 0.0 |
| R | 3 | 40 | 4200.654 | 0,072 | 0.0 | R | 3 | 39 | 4200,330 | 0,084 | 0.0 |
| R | 3 | 38 | 4200.206 | 0,069 | 0.0 | R | 3 | 37 | 4199,871 | 0,070 | 0.0 |
| R | 3 | 36 | 4199.709 | 0,076 | 0.0 | R | 3 | 35 | 4199,357 | 0,068 | 0.0 |
| R | 3 | 34 | 4199.122 | 0,051 | 0.0 | R | 3 | 33 | 4198,772 | 0,057 | 0.0 |
| R | 3 | 32 | 4198.494 | 0,046 | 0.0 | R | 3 | 31 | 4198,120 | 0,043 | 0.0 |
| R | 3 | 30 | 4197.805 | 0,040 | 0.0 | R | 3 | 29 | 4197,411 | 0,036 | 0.0 |
| R | 3 | 28 | 4197.056 | 0,033 | 0.0 | R | 3 | 27 | 4196,632 | 0,022 | 0.0 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| R | 3 | 26 | 4196.243 | 0,024 | 0.0 | R | 3 | 25 | 4195,800 | 0,018 | 0.0 |
| R | 3 | 24 | 4195.378 | 0,023 | 0.0 | R | 3 | 23 | 4194,892 | 0,001 | 0.0 |
| R | 3 | 22 | 4194.445 | 0,016 | 0.0 | R | 3 | 21 | 4193,940 | 0,002 | 0.0 |
| R | 3 | 20 | 4193.447 | 0,006 | 0.0 | R | 3 | 19 | 4192,928 | 0,007 | 0.0 |
| R | 3 | 18 | 4192.415 | 0,023 | 0.0 | R | 3 | 17 | 4191,843 | 0,001 | 0.0 |
| R | 3 | 16 | 4191.289 | 0,009 | 0.0 | R | 3 | 15 | 4190,697 | -0,003 | 0.0 |
| R | 3 | 14 | 4190.123 | 0,016 | 0.0 | R | 3 | 13 | 4189,502 | 0,006 | 0.0 |
| R | 3 | 12 | 4188.878 | 0,007 | 0.0 | R | 3 | 11 | 4188,237 | 0,008 | 0.0 |
| R | 3 | 10 | 4187.571 | -0,001 | 0.0 | R | 3 | 9 | 4186,890 | -0,010 | 0.0 |
| R | 3 | 8 | 4186.215 | 0,003 | 0.0 | R | 3 | 7 | 4185,505 | -0,002 | 0.0 |
| R | 3 | 6 | 4184.794 | 0,006 | 0.7 | R | 3 | 5 | 4184,054 | 0,001 | 1.0 |
| R | 3 | 4 | 4183.303 | -0,000 | 1.0 | R | 3 | 3 | 4182,537 | 0,001 | 1.0 |
| R | 4 | 47 | 4200.845 | -0,081 | 0.0 | R | 4 | 46 | 4200,775 | -0,081 | 0.0 |
| R | 4 | 45 | 4200.654 | -0,075 | 0.1 | R | 4 | 44 | 4200,551 | -0,070 | 0.1 |
| R | 4 | 43 | 4200.417 | -0,052 | 0.0 | R | 4 | 42 | 4200,284 | -0,041 | 0.0 |
| R | 4 | 41 | 4200.112 | -0,034 | 0.0 | R | 4 | 40 | 4199,949 | -0,017 | 0.0 |
| R | 4 | 39 | 4199.730 | -0,028 | 0.0 | R | 4 | 38 | 4199,519 | -0,027 | 0.0 |
| R | 4 | 37 | 4199.293 | -0,015 | 0.1 | R | 4 | 36 | 4199,042 | -0,021 | 0.0 |
| R | 4 | 35 | 4198.772 | -0,023 | 0.3 | R | 4 | 34 | 4198,494 | -0,023 | 0.0 |
| R | 4 | 33 | 4198.199 | -0,020 | 0.0 | R | 4 | 32 | 4197,929 | 0,020 | 0.0 |
| R | 4 | 31 | 4197.587 | 0,008 | 0.0 | R | 4 | 30 | 4197,252 | 0,015 | 0.0 |
| R | 4 | 29 | 4196.875 | -0,002 | 0.1 | R | 4 | 28 | 4196,522 | 0,019 | 0.0 |
| R | 4 | 27 | 4196.105 | -0,007 | 0.1 | R | 4 | 26 | 4195,717 | 0,010 | 0.0 |
| R | 4 | 25 | 4195.291 | 0,007 | 0.1 | R | 4 | 24 | 4194,855 | 0,008 | 0.0 |
| R | 4 | 23 | 4194.393 | -0,000 | 0.1 | R | 4 | 22 | 4193,930 | 0,005 | 0.0 |
| R | 4 | 21 | 4193.447 | 0,007 | 0.0 | R | 4 | 20 | 4192,928 | -0,012 | 0.0 |
| R | 4 | 19 | 4192.415 | -0,009 | 0.0 | R | 4 | 18 | 4191,887 | -0,005 | 0.0 |
| R | 4 | 17 | 4191.338 | -0,007 | 0.1 | R | 4 | 16 | 4190,780 | -0,002 | 0.7 |
| R | 4 | 15 | 4190.202 | -0,002 | 1.0 | R | 4 | 14 | 4189,603 | -0,006 | 0.0 |
| R | 4 | 13 | 4188.986 | -0,013 | 0.0 | R | 4 | 12 | 4188,360 | -0,013 | 0.0 |
| R | 4 | 11 | 4187.717 | -0,015 | 0.0 | R | 4 | 10 | 4187,073 | -0,002 | 0.0 |
| R | 4 | 9 | 4186.407 | 0,004 | 0.0 | R | 4 | 8 | 4185,706 | -0,008 | 0.0 |
| R | 4 | 7 | 4185.007 | -0,003 | 0.0 | R | 4 | 6 | 4184,288 | -0,003 | 0.5 |
| R | 4 | 5 | 4183.553 | -0,002 | 0.1 | R | 4 | 4 | 4182,791 | -0,013 | 0.0 |
| R | 5 | 40 | 4199.357 | 0,035 | 0.0 | R | 5 | 39 | 4199,122 | 0,001 | 0.0 |
| R | 5 | 38 | 4198.929 | 0,026 | 0.0 | R | 5 | 37 | 4198,688 | 0,018 | 0.0 |
| R | 5 | 36 | 4198.449 | 0,029 | 0.0 | R | 5 | 35 | 4198,178 | 0,022 | 0.0 |
| R | 5 | 34 | 4197.901 | 0,026 | 0.0 | R | 5 | 33 | 4197,587 | 0,009 | 0.0 |
| R | 5 | 32 | 4197.291 | 0,025 | 0.0 | R | 5 | 31 | 4196,952 | 0,014 | 0.7 |
| R | 5 | 30 | 4196.604 | 0,010 | 0.0 | R | 5 | 29 | 4196,243 | 0,008 | 0.0 |
| R | 5 | 28 | 4195.875 | 0,015 | 0.0 | R | 5 | 27 | 4195,472 | 0,003 | 0.0 |
| R | 5 | 26 | 4195.074 | 0,012 | 0.3 | R | 5 | 25 | 4194,653 | 0,014 | 0.1 |
| R | 5 | 24 | 4194.217 | 0,016 | 0.0 | R | 5 | 23 | 4193,751 | 0,004 | 0.3 |
| R | 5 | 22 | 4193.278 | 0,001 | 0.0 | R | 5 | 21 | 4192,798 | 0,005 | 0.0 |
| R | 5 | 20 | 4192.293 | 0,002 | 1.0 | R | 5 | 19 | 4191,784 | 0,010 | 0.0 |
| R | 5 | 18 | 4191.247 | 0,005 | 0.0 | R | 5 | 17 | 4190,697 | 0,003 | 0.0 |
| R | 5 | 16 | 4190.123 | -0,007 | 0.0 | R | 5 | 15 | 4189,545 | -0,006 | 0.0 |
| R | 5 | 14 | 4188.949 | -0,007 | 0.0 | R | 5 | 13 | 4188,336 | -0,009 | 0.0 |
| R | 5 | 12 | 4187.717 | -0,001 | 0.0 | R | 5 | 11 | 4187,073 | -0,004 | 0.0 |
| R | 5 | 10 | 4186.406 | -0,012 | 0.0 | R | 5 | 9 | 4185,743 | -0,002 | 0.0 |
| R | 5 | 8 | 4185.061 | 0,004 | 0.0 | R | 5 | 7 | 4184,354 | 0,002 | 0.0 |
| R | 5 | 6 | 4183.624 | -0,007 | 0.0 | R | 5 | 5 | 4182,892 | -0,004 | 0.0 |
| R | 6 | 40 | 4198.600 | 0,033 | 0.0 | R | 6 | 39 | 4198,374 | 0,012 | 0.0 |
| R | 6 | 38 | 4198.178 | 0,037 | 0.0 | R | 6 | 37 | 4197,929 | 0,024 | 0.0 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| R | 6 | 36 | 4197,675 | 0,023 | 0.0 | R | 6 | 35 | 4197,411 | 0,027 | 0.0 |
| R | 6 | 34 | 4197,118 | 0,017 | 0.0 | R | 6 | 33 | 4196,824 | 0,023 | 0.0 |
| R | 6 | 32 | 4196,522 | 0,037 | 0.0 | R | 6 | 31 | 4196,180 | 0,025 | 0.0 |
| R | 6 | 30 | 4195,837 | 0,030 | 0.0 | R | 6 | 29 | 4195,472 | 0,026 | 0.0 |
| R | 6 | 28 | 4195,074 | 0,007 | 0.0 | R | 6 | 27 | 4194,689 | 0,016 | 0.0 |
| R | 6 | 26 | 4194,279 | 0,015 | 0.0 | R | 6 | 25 | 4193,837 | -0,002 | 0.0 |
| R | 6 | 24 | 4193,397 | -0,001 | 0.0 | R | 6 | 23 | 4192,928 | -0,013 | 0.0 |
| R | 6 | 22 | 4192,473 | 0,004 | 0.0 | R | 6 | 21 | 4191,975 | -0,007 | 0.5 |
| R | 6 | 20 | 4191,480 | 0,002 | 0.7 | R | 6 | 19 | 4190,947 | -0,012 | 0.0 |
| R | 6 | 18 | 4190,426 | 0,002 | 0.0 | R | 6 | 17 | 4189,888 | 0,014 | 0.0 |
| R | 6 | 16 | 4189,317 | 0,009 | 0.3 | R | 6 | 15 | 4188,729 | 0,002 | 0.7 |
| R | 6 | 14 | 4188,138 | 0,008 | 0.0 | R | 6 | 13 | 4187,522 | 0,004 | 0.0 |
| R | 6 | 12 | 4186,890 | 0,001 | 0.0 | R | 6 | 11 | 4186,237 | -0,009 | 0.1 |
| R | 6 | 10 | 4185,582 | -0,005 | 0.3 | R | 6 | 9 | 4184,909 | -0,003 | 0.2 |
| R | 6 | 8 | 4184,223 | 0,002 | 0.2 | R | 6 | 7 | 4183,516 | 0,001 | 0.1 |
| R | 6 | 6 | 4182,815 | 0,021 | 0.0 | | | | | | |

# FREQUENCIES FOR THE (1,0,1) BAND OF 15NO2

| | K | N | OBS | O-C | WT | | K | N | OBS | O-C | WT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| P | 0 | 46 | 2809.729 | 0.020 | 0.1 | P | 0 | 44 | 2812.270 | -0.004 | 0.0 |
| P | 0 | 42 | 2814.805 | -0.000 | 0.3 | P | 0 | 40 | 2817.285 | -0.010 | 0.0 |
| P | 0 | 38 | 2819.745 | 0.001 | 0.1 | P | 0 | 36 | 2822.155 | 0.004 | 0.1 |
| P | 0 | 34 | 2824.518 | 0.001 | 0.2 | P | 0 | 32 | 2826.848 | 0.006 | 0.5 |
| P | 0 | 30 | 2829.133 | 0.005 | 0.5 | P | 0 | 28 | 2831.378 | 0.006 | 1.0 |
| P | 0 | 26 | 2833.589 | 0.004 | 1.0 | P | 0 | 24 | 2835.752 | 0.008 | 1.0 |
| P | 0 | 22 | 2837.873 | 0.002 | 0.1 | P | 0 | 20 | 2839.968 | 0.009 | 1.0 |
| P | 0 | 18 | 2842.016 | 0.007 | 1.0 | P | 0 | 16 | 2844.026 | 0.006 | 1.0 |
| P | 0 | 14 | 2845.998 | 0.005 | 1.0 | P | 0 | 12 | 2847.935 | 0.008 | 1.0 |
| P | 0 | 10 | 2849.833 | 0.011 | 1.0 | P | 0 | 8 | 2851.685 | 0.007 | 1.0 |
| P | 0 | 6 | 2853.501 | 0.005 | 0.2 | P | 0 | 4 | 2855.281 | 0.008 | 0.1 |
| P | 0 | 2 | 2857.014 | 0.004 | 0.0 | P | 1 | 47 | 2808.373 | -0.023 | 0.0 |
| P | 1 | 46 | 2809.026 | -0.021 | 0.1 | P | 1 | 45 | 2810.981 | -0.010 | 0.2 |
| P | 1 | 44 | 2811.614 | -0.014 | 0.1 | P | 1 | 43 | 2813.517 | -0.028 | 0.0 |
| P | 1 | 42 | 2814.160 | -0.010 | 0.3 | P | 1 | 41 | 2816.047 | -0.011 | 0.2 |
| P | 1 | 40 | 2816.662 | -0.010 | 0.0 | P | 1 | 39 | 2818.524 | -0.007 | 0.1 |
| P | 1 | 38 | 2819.130 | -0.006 | 0.1 | P | 1 | 37 | 2820.956 | -0.007 | 0.5 |
| P | 1 | 36 | 2821.570 | 0.008 | 0.0 | P | 1 | 35 | 2823.354 | 0.001 | 0.5 |
| P | 1 | 34 | 2823.945 | -0.003 | 0.1 | P | 1 | 33 | 2825.700 | -0.004 | 0.5 |
| P | 1 | 32 | 2826.297 | 0.001 | 0.5 | P | 1 | 31 | 2828.013 | 0.000 | 1.0 |
| P | 1 | 30 | 2828.606 | 0.001 | 1.0 | P | 1 | 29 | 2830.280 | -0.001 | 1.0 |
| P | 1 | 28 | 2830.872 | -0.004 | 1.0 | P | 1 | 27 | 2832.510 | 0.002 | 1.0 |
| P | 1 | 26 | 2833.112 | 0.003 | 0.5 | P | 1 | 25 | 2834.697 | 0.002 | 1.0 |
| P | 1 | 24 | 2835.299 | -0.003 | 0.1 | P | 1 | 23 | 2836.845 | 0.004 | 1.0 |
| P | 1 | 22 | 2837.457 | 0.000 | 1.0 | P | 1 | 21 | 2838.946 | -0.000 | 1.0 |
| P | 1 | 20 | 2839.575 | 0.002 | 1.0 | P | 1 | 19 | 2841.007 | -0.003 | 1.0 |
| P | 1 | 18 | 2841.670 | 0.020 | 0.0 | P | 1 | 17 | 2843.033 | -0.001 | 1.0 |
| P | 1 | 16 | 2843.688 | 0.000 | 0.0 | P | 1 | 15 | 2845.016 | -0.000 | 1.0 |
| P | 1 | 14 | 2845.674 | -0.013 | 0.0 | P | 1 | 13 | 2846.957 | -0.001 | 1.0 |
| P | 1 | 12 | 2847.648 | 0.001 | 1.0 | P | 1 | 11 | 2848.860 | 0.002 | 1.0 |
| P | 1 | 10 | 2849.564 | -0.003 | 1.0 | P | 1 | 9 | 2850.713 | -0.005 | 1.0 |
| P | 1 | 8 | 2851.451 | 0.003 | 1.0 | P | 1 | 7 | 2852.534 | -0.002 | 1.0 |
| P | 1 | 6 | 2853.293 | 0.004 | 0.3 | P | 1 | 5 | 2854.313 | 0.000 | 0.1 |
| P | 1 | 4 | 2855.087 | -0.004 | 1.0 | P | 1 | 3 | 2856.047 | -0.001 | 0.1 |
| P | 1 | 2 | 2856.863 | 0.012 | 0.0 | P | 2 | 48 | 2805.985 | -0.014 | 0.0 |
| P | 2 | 47 | 2807.601 | -0.005 | 0.1 | P | 2 | 46 | 2808.602 | -0.025 | 0.1 |
| P | 2 | 45 | 2810.207 | 0.001 | 0.1 | P | 2 | 44 | 2811.201 | -0.016 | 0.1 |
| P | 2 | 43 | 2812.762 | -0.005 | 0.3 | P | 2 | 42 | 2813.760 | -0.011 | 0.1 |
| P | 2 | 41 | 2815.286 | -0.002 | 0.3 | P | 2 | 40 | 2816.281 | -0.005 | 0.0 |
| P | 2 | 39 | 2817.784 | 0.014 | 0.0 | P | 2 | 38 | 2818.762 | -0.002 | 0.1 |
| P | 2 | 37 | 2820.211 | 0.000 | 0.1 | P | 2 | 36 | 2821.200 | -0.003 | 0.1 |
| P | 2 | 35 | 2822.611 | -0.002 | 0.5 | P | 2 | 34 | 2823.599 | -0.004 | 0.2 |
| P | 2 | 33 | 2824.973 | -0.002 | 0.1 | P | 2 | 32 | 2825.960 | -0.004 | 0.3 |
| P | 2 | 31 | 2827.286 | -0.010 | 0.1 | P | 2 | 30 | 2828.286 | -0.001 | 0.5 |
| P | 2 | 29 | 2829.573 | -0.005 | 1.0 | P | 2 | 28 | 2830.563 | -0.007 | 0.3 |
| P | 2 | 27 | 2831.815 | -0.006 | 1.0 | P | 2 | 26 | 2832.809 | -0.003 | 0.5 |
| P | 2 | 25 | 2834.012 | -0.011 | 0.3 | P | 2 | 24 | 2835.013 | -0.001 | 1.0 |
| P | 2 | 23 | 2836.178 | -0.007 | 1.0 | P | 2 | 22 | 2837.167 | -0.007 | 1.0 |
| P | 2 | 21 | 2838.303 | -0.005 | 1.0 | P | 2 | 20 | 2839.286 | -0.007 | 1.0 |
| P | 2 | 19 | 2840.377 | -0.012 | 0.1 | P | 2 | 18 | 2841.361 | -0.008 | 1.0 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| P | 2 | 17 | 2842.415 | -0,016 | 0.1 | P | 2 | 16 | 2843,389 | -0,014 | 0.1 |
| P | 2 | 15 | 2844;422 | -0,011 | 1.0 | P | 2 | 14 | 2845,384 | -0.011 | 1.0 |
| P | 2 | 13 | 2846.385 | -0,010 | 1.0 | P | 2 | 12 | 2847,336 | -0.009 | 0.5 |
| P | 2 | 11 | 2848.303 | -0,013 | 1.0 | P | 2 | 10 | 2849,239 | -0.013 | 0.5 |
| P | 2 | 9 | 2850.183 | -0,013 | 1.0 | P | 2 | 8 | 2851,101 | -0,015 | 1.0 |
| P | 2 | 7 | 2852.027 | -0,010 | 1.0 | P | 2 | 6 | 2852,953 | 0,014 | 1,0 |
| P | 2 | 5 | 2853.825 | -0,010 | 0.1 | P | 2 | 4 | 2854,697 | -0.023 | 0.0 |
| P | 2 | 3 | 2855;579 | -0,015 | 0,0 | P | 3 | 48 | 2805,447 | 0,033 | 0.0 |
| P | 3 | 47 | 2806,828 | 0,047 | 0.1 | P | 3 | 46 | 2808,074 | 0,032 | 0.1 |
| P | 3 | 45 | 2809;428 | 0,042 | 0.1 | P | 3 | 44 | 2810,667 | 0,035 | 0.1 |
| P | 3 | 43 | 2811.988 | 0,036 | 0.3 | P | 3 | 42 | 2813,220 | 0,037 | 0.3 |
| P | 3 | 41 | 2814;517 | 0,039 | 0.2 | P | 3 | 40 | 2815,728 | 0,033 | 0.0 |
| P | 3 | 39 | 2817;000 | 0,035 | 0.1 | P | 3 | 38 | 2818,200 | 0,032 | 0.1 |
| P | 3 | 37 | 2819;444 | 0,031 | 0.1 | P | 3 | 36 | 2820,632 | 0,032 | 0.1 |
| P | 3 | 35 | 2821;851 | 0,029 | 0.2 | P | 3 | 34 | 2823,023 | 0,031 | 0.5 |
| P | 3 | 33 | 2824.223 | 0,034 | 0.3 | P | 3 | 32 | 2825,376 | 0,031 | 0.1 |
| P | 3 | 31 | 2826.550 | 0,032 | 0.1 | P | 3 | 30 | 2827,680 | 0.023 | 0.1 |
| P | 3 | 29 | 2828.819 | 0,012 | 0.1 | P | 3 | 28 | 2829,941 | 0,013 | 0.0 |
| P | 3 | 27 | 2831.071 | 0,016 | 0.1 | P | 3 | 26 | 2832,172 | 0,013 | 0.1 |
| P | 3 | 25 | 2833.293 | 0,029 | 0.1 | P | 3 | 24 | 2834,375 | 0,026 | 0.1 |
| P | 3 | 23 | 2835.453 | 0,021 | 0.1 | P | 3 | 22 | 2836,515 | 0.017 | 0.1 |
| P | 3 | 21 | 2837.570 | 0,010 | 0.1 | P | 3 | 20 | 2838,615 | 0,009 | 0.1 |
| P | 3 | 19 | 2839.647 | 0,001 | 0.1 | P | 3 | 18 | 2840,671 | -0,003 | 0.1 |
| P | 3 | 17 | 2841.670 | -0,023 | 0.0 | P | 3 | 16 | 2842,685 | -0.015 | 0.0 |
| P | 3 | 15 | 2843.688 | -0,010 | 0.0 | P | 3 | 14 | 2844,693 | 0,008 | 0.0 |
| P | 3 | 13 | 2845.674 | 0,012 | 0.0 | P | 3 | 12 | 2846,629 | -0,001 | 0.2 |
| P | 3 | 11 | 2847;585 | -0,001 | 0.3 | P | 3 | 10 | 2848,531 | -0.001 | 1.0 |
| P | 3 | 9 | 2849.465 | -0,004 | 0,7 | P | 3 | 8 | 2850,395 | 0,000 | 0.0 |
| P | 3 | 7 | 2851;306 | -0,004 | 0,7 | P | 3 | 6 | 2852,216 | 0,001 | 0.0 |
| P | 3 | 5 | 2853.101 | -0,010 | 0.0 | P | 3 | 4 | 2853,984 | -0,011 | 0.0 |
| P | 4 | 37 | 2818;365 | -0,015 | 0,0 | P | 4 | 36 | 2819,569 | -0,019 | 0.1 |
| P | 4 | 35 | 2820.765 | -0,023 | 0.1 | P | 4 | 34 | 2821,948 | -0.030 | 0.1 |
| P | 4 | 33 | 2823;122 | -0,036 | 0.1 | P | 4 | 32 | 2824,294 | -0,033 | 0.1 |
| P | 4 | 31 | 2825;452 | -0,034 | 0,2 | P | 4 | 30 | 2826,618 | -0,018 | 0.5 |
| P | 4 | 29 | 2827.749 | -0,026 | 0.3 | P | 4 | 28 | 2828,879 | -0,026 | 0,2 |
| P | 4 | 27 | 2830.007 | -0,018 | 0,2 | P | 4 | 26 | 2831,116 | -0,018 | 0.1 |
| P | 4 | 25 | 2832;214 | -0,019 | 0,1 | P | 4 | 24 | 2833,293 | -0,029 | 0.1 |
| P | 4 | 23 | 2834.375 | -0,026 | 0.1 | P | 4 | 22 | 2835,453 | -0.017 | 0.1 |
| P | 4 | 21 | 2836.515 | -0,013 | 0.1 | P | 4 | 20 | 2837,570 | -0,008 | 0.1 |
| P | 4 | 19 | 2838;615 | -0,001 | 0.1 | P | 4 | 18 | 2839,647 | 0,003 | 0.1 |
| P | 4 | 17 | 2840.671 | 0,009 | 0.1 | P | 4 | 16 | 2841,706 | 0,036 | 0.0 |
| P | 4 | 15 | 2842;685 | 0,018 | 0.0 | P | 4 | 14 | 2843,688 | 0,034 | 0.0 |
| P | 4 | 13 | 2844;640 | 0,008 | 0.0 | P | 4 | 12 | 2845,611 | 0,012 | 0,3 |
| P | 4 | 11 | 2846.573 | 0,017 | 0,3 | P | 4 | 10 | 2847,520 | 0,017 | 0.5 |
| P | 4 | 9 | 2848;460 | 0,022 | 0.1 | P | 4 | 8 | 2849,385 | 0.021 | 0.0 |
| P | 4 | 7 | 2850;295 | 0,015 | 0.0 | P | 4 | 6 | 2851,215 | 0,029 | 0.0 |
| P | 4 | 5 | 2852.107 | 0,026 | 0,0 | P | 5 | 35 | 2819,569 | 0,022 | 0.0 |
| P | 5 | 34 | 2820;765 | 0,028 | 0.0 | P | 5 | 33 | 2821,948 | 0,031 | 0,0 |
| P | 5 | 32 | 2823;122 | 0,036 | 0.0 | P | 5 | 31 | 2824,294 | 0,048 | 0,0 |
| P | 5 | 30 | 2825;414 | 0,019 | 0,0 | P | 5 | 29 | 2826,550 | 0,015 | 0.0 |
| P | 5 | 28 | 2827.680 | 0,016 | 0,0 | P | 5 | 27 | 2828,796 | 0,012 | 0.0 |
| P | 5 | 26 | 2829.901 | 0,009 | 0,0 | P | 5 | 25 | 2831,007 | 0,015 | 0.2 |
| P | 5 | 24 | 2832.094 | 0,013 | 0,2 | P | 5 | 23 | 2833,171 | 0,010 | 0.3 |
| P | 5 | 22 | 2834;239 | 0,009 | 0.3 | P | 5 | 21 | 2835,299 | 0,011 | 0.0 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| P | 5 | 20 | 2836,343 | 0,006 | 1,0 | P | 5 | 19 | 2837,380 | 0,004 | 1,0 |
| P | 5 | 18 | 2838,402 | -0,002 | 1,0 | P | 5 | 17 | 2839,422 | -0,001 | 1,0 |
| P | 5 | 16 | 2840,425 | -0,005 | 0,0 | P | 5 | 15 | 2841,423 | -0,005 | 0,7 |
| P | 5 | 14 | 2842,415 | -0,001 | 0,0 | P | 5 | 13 | 2843,389 | -0,004 | 0,0 |
| P | 5 | 12 | 2844,352 | -0,009 | 0,3 | P | 5 | 11 | 2845,307 | -0,011 | 0,5 |
| P | 5 | 10 | 2846,253 | -0,012 | 0,3 | P | 5 | 9 | 2847,173 | -0,028 | 0,0 |
| P | 5 | 8 | 2848,137 | 0,009 | 0,0 | P | 5 | 7 | 2849,036 | -0,007 | 0,0 |
| Q | 1 | 2 | 2858,465 | -0,002 | 0,1 | Q | 1 | 1 | 2858,585 | -0,002 | 0,2 |
| Q | 2 | 8 | 2857,764 | -0,008 | 0,0 | Q | 2 | 7 | 2857,852 | -0,023 | 0,0 |
| Q | 2 | 6 | 2857,922 | -0,013 | 0,0 | Q | 2 | 5 | 2857,994 | -0,009 | 0,0 |
| Q | 2 | 4 | 2858,039 | -0,012 | 0,0 | Q | 2 | 3 | 2858,101 | 0,007 | 0,0 |
| Q | 2 | 2 | 2858,101 | -0,023 | 0,0 | Q | 3 | 13 | 2856,495 | -0,001 | 0,0 |
| Q | 3 | 12 | 2856,633 | 0,005 | 0,0 | Q | 3 | 11 | 2856,751 | -0,001 | 0,0 |
| Q | 3 | 10 | 2856,863 | -0,002 | 0,0 | Q | 3 | 9 | 2856,975 | 0,007 | 0,0 |
| Q | 3 | 8 | 2857,060 | -0,000 | 0,0 | Q | 3 | 7 | 2857,140 | -0,002 | 0,1 |
| Q | 3 | 6 | 2857,216 | 0,001 | 0,2 | Q | 3 | 5 | 2857,285 | 0,008 | 0,0 |
| Q | 3 | 4 | 2857,336 | 0,008 | 0,0 | Q | 3 | 3 | 2857,367 | -0,002 | 0,0 |
| Q | 4 | 10 | 2855,856 | 0,019 | 0,2 | Q | 4 | 9 | 2855,956 | 0,017 | 0,2 |
| Q | 4 | 8 | 2856,047 | 0,015 | 0,0 | Q | 4 | 7 | 2856,133 | 0,019 | 0,5 |
| Q | 4 | 6 | 2856,210 | 0,023 | 0,5 | Q | 4 | 5 | 2856,280 | 0,031 | 0,1 |
| Q | 4 | 4 | 2856,331 | 0,031 | 0,2 | Q | 5 | 11 | 2854,473 | -0,016 | 0,1 |
| Q | 5 | 10 | 2854,592 | -0,010 | 0,1 | Q | 5 | 9 | 2854,697 | -0,008 | 0,0 |
| Q | 5 | 8 | 2854,787 | -0,011 | 0,1 | Q | 5 | 7 | 2854,864 | -0,016 | 0,2 |
| Q | 5 | 6 | 2854,938 | -0,015 | 0,1 | Q | 5 | 5 | 2854,999 | -0,015 | 0,2 |
| R | 0 | 46 | 2885,570 | -0,034 | 0,1 | R | 0 | 44 | 2884,981 | 0,005 | 0,2 |
| R | 0 | 42 | 2884,306 | 0,001 | 0,3 | R | 0 | 40 | 2883,590 | 0,000 | 0,0 |
| R | 0 | 38 | 2882,826 | -0,005 | 0,0 | R | 0 | 36 | 2882,024 | -0,003 | 1,0 |
| R | 0 | 34 | 2881,179 | 0,001 | 1,0 | R | 0 | 32 | 2880,284 | 0,002 | 1,0 |
| R | 0 | 30 | 2879,342 | 0,002 | 1,0 | R | 0 | 28 | 2878,356 | 0,006 | 0,1 |
| R | 0 | 26 | 2877,315 | 0,002 | 0,3 | R | 0 | 24 | 2876,239 | 0,012 | 0,1 |
| R | 0 | 22 | 2875,099 | 0,006 | 1,0 | R | 0 | 20 | 2873,916 | 0,006 | 1,0 |
| R | 0 | 18 | 2872,684 | 0,007 | 1,0 | R | 0 | 16 | 2871,407 | 0,006 | 1,0 |
| R | 0 | 14 | 2870,082 | 0,007 | 1,0 | R | 0 | 12 | 2868,711 | 0,008 | 0,1 |
| R | 0 | 10 | 2867,295 | 0,009 | 0,0 | R | 0 | 8 | 2865,819 | -0,004 | 0,0 |
| R | 0 | 6 | 2864,319 | 0,001 | 0,0 | R | 0 | 4 | 2862,772 | 0,005 | 0,1 |
| R | 0 | 2 | 2861,175 | 0,001 | 0,5 | R | 0 | 0 | 2859,544 | 0,004 | 0,1 |
| R | 1 | 47 | 2885,741 | -0,009 | 0,0 | R | 1 | 46 | 2886,689 | -0,020 | 0,2 |
| R | 1 | 45 | 2885,129 | 0,005 | 0,0 | R | 1 | 44 | 2886,037 | 0,003 | 0,0 |
| R | 1 | 43 | 2884,443 | -0,013 | 0,1 | R | 1 | 42 | 2885,293 | -0,014 | 0,1 |
| R | 1 | 41 | 2883,711 | -0,030 | 0,0 | R | 1 | 40 | 2884,519 | -0,012 | 1,0 |
| R | 1 | 39 | 2882,980 | -0,003 | 0,0 | R | 1 | 38 | 2883,711 | 0,006 | 0,0 |
| R | 1 | 37 | 2882,169 | -0,012 | 0,3 | R | 1 | 36 | 2882,826 | -0,005 | 0,0 |
| R | 1 | 35 | 2881,332 | -0,002 | 1,0 | R | 1 | 34 | 2881,908 | -0,001 | 0,1 |
| R | 1 | 33 | 2880,437 | -0,006 | 0,5 | R | 1 | 32 | 2880,944 | 0,005 | 0,0 |
| R | 1 | 31 | 2879,495 | -0,012 | 0,0 | R | 1 | 30 | 2879,914 | -0,008 | 0,1 |
| R | 1 | 29 | 2878,539 | 0,012 | 0,0 | R | 1 | 28 | 2878,859 | 0,000 | 1,0 |
| R | 1 | 27 | 2877,501 | -0,001 | 0,0 | R | 1 | 26 | 2877,754 | 0,003 | 0,2 |
| R | 1 | 25 | 2876,420 | -0,014 | 0,0 | R | 1 | 24 | 2876,599 | 0,001 | 1,0 |
| R | 1 | 23 | 2875,323 | 0,003 | 0,1 | R | 1 | 22 | 2875,399 | -0,001 | 1,0 |
| R | 1 | 21 | 2874,150 | -0,013 | 0,0 | R | 1 | 20 | 2874,150 | -0,009 | 0,0 |
| R | 1 | 19 | 2872,951 | -0,011 | 0,0 | R | 1 | 18 | 2872,864 | -0,010 | 0,0 |
| R | 1 | 17 | 2871,727 | 0,010 | 0,0 | R | 1 | 16 | 2871,538 | -0,009 | 0,0 |
| R | 1 | 15 | 2870,436 | 0,007 | 0,0 | R | 1 | 14 | 2870,170 | -0,006 | 0,0 |
| R | 1 | 13 | 2869,097 | 0,000 | 1,0 | R | 1 | 12 | 2868,765 | 0,001 | 0,0 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| R | 1 | 11 | 2867.717 | -0,004 | 1,0 | R | 1 | 10 | 2867,295 | -0,014 | 0.0 |
| R | 1 | 9 | 2866,303 | -0,000 | 1,0 | R | 1 | 8 | 2865,819 | 0,006 | 0.0 |
| R | 1 | 7 | 2864,839 | -0,003 | 1,0 | R | 1 | 6 | 2864,276 | 0,001 | 0.0 |
| R | 1 | 5 | 2863.336 | -0,002 | 1,0 | R | 1 | 4 | 2862,696 | -0.002 | 1.0 |
| R | 1 | 3 | 2861,790 | -0,001 | 1,0 | R | 1 | 2 | 2861,079 | 0,001 | 0.7 |
| R | 1 | 1 | 2860,207 | 0,004 | 0,0 | R | 2 | 47 | 2886,137 | 0,002 | 0.1 |
| R | 2 | 46 | 2886,820 | -0,018 | 0,0 | R | 2 | 45 | 2885,467 | -0,008 | 0.3 |
| R | 2 | 44 | 2886.037 | -0,032 | 0,0 | R | 2 | 43 | 2884,765 | -0.005 | 0.1 |
| R | 2 | 42 | 2885,241 | -0,013 | 0,1 | R | 2 | 41 | 2884,025 | 0,006 | 0.1 |
| R | 2 | 40 | 2884.388 | -0,006 | 0,0 | R | 2 | 39 | 2883,239 | 0,014 | 0.2 |
| R | 2 | 38 | 2883.480 | -0,011 | 0,3 | R | 2 | 37 | 2882,385 | 0,000 | 0.3 |
| R | 2 | 36 | 2882,536 | -0,011 | 0,3 | R | 2 | 35 | 2881,488 | -0,012 | 0.0 |
| R | 2 | 34 | 2881,545 | -0,015 | 0,0 | R | 2 | 33 | 2880,587 | 0,017 | 0.0 |
| R | 2 | 32 | 2880,531 | -0,003 | 0,0 | R | 2 | 31 | 2879,587 | -0,009 | 0.1 |
| R | 2 | 30 | 2879.455 | -0,013 | 0,0 | R | 2 | 29 | 2878,584 | 0,005 | 0.0 |
| R | 2 | 28 | 2878,356 | -0,008 | 0,1 | R | 2 | 27 | 2877,501 | -0,016 | 0.0 |
| R | 2 | 26 | 2877,224 | 0,001 | 0,2 | R | 2 | 25 | 2876,420 | 0,008 | 0.0 |
| R | 2 | 24 | 2874.039 | -0,005 | 1,0 | R | 2 | 23 | 2875,260 | -0,003 | 0.0 |
| R | 2 | 22 | 2874,822 | -0,007 | 1,0 | R | 2 | 21 | 2874,067 | -0.004 | 0.0 |
| R | 2 | 20 | 2873,557 | -0,020 | 0,0 | R | 2 | 19 | 2872,817 | -0,018 | 0.0 |
| R | 2 | 18 | 2872,281 | -0,008 | 0,7 | R | 2 | 17 | 2871,538 | -0,019 | 0.0 |
| R | 2 | 16 | 2870,953 | -0,011 | 1,0 | R | 2 | 15 | 2870,212 | -0,024 | 0.0 |
| R | 2 | 14 | 2869.598 | -0,003 | 0,1 | R | 2 | 13 | 2868,857 | -0,016 | 0.0 |
| R | 2 | 12 | 2868,179 | -0,023 | 0,0 | R | 2 | 11 | 2867,460 | -0,007 | 0.0 |
| R | 2 | 10 | 2866.756 | -0,008 | 0,0 | R | 2 | 9 | 2866,019 | -0,001 | 0.0 |
| R | 2 | 8 | 2865,283 | -0,005 | 0,0 | R | 2 | 7 | 2864,523 | -0,007 | 0.0 |
| R | 2 | 6 | 2863.766 | -0,007 | 0,0 | R | 2 | 5 | 2862,985 | -0,013 | 0.0 |
| R | 2 | 4 | 2862,202 | -0,016 | 0,0 | R | 2 | 3 | 2861,418 | -0,008 | 0.0 |
| R | 2 | 2 | 2860.608 | -0,015 | 0,0 | R | 3 | 45 | 2885,129 | 0,034 | 0.0 |
| R | 3 | 44 | 2884.981 | 0,025 | 0,0 | R | 3 | 43 | 2884,388 | 0,037 | 0.0 |
| R | 3 | 42 | 2884.163 | 0,018 | 0,2 | R | 3 | 41 | 2883,590 | 0,025 | 0.0 |
| R | 3 | 40 | 2883.326 | 0,027 | 0,5 | R | 3 | 39 | 2882,778 | 0,042 | 0.0 |
| R | 3 | 38 | 2882.452 | 0,036 | 0,1 | R | 3 | 37 | 2881,908 | 0,043 | 0.1 |
| R | 3 | 36 | 2881.545 | 0,048 | 0,0 | R | 3 | 35 | 2880,981 | 0,031 | 0.0 |
| R | 3 | 34 | 2880,568 | 0,026 | 0,0 | R | 3 | 33 | 2880,028 | 0,034 | 0.1 |
| R | 3 | 32 | 2879,587 | 0,039 | 0,1 | R | 3 | 31 | 2879,026 | 0,029 | 1.0 |
| R | 3 | 30 | 2878.539 | 0,022 | 0,0 | R | 3 | 29 | 2877,984 | 0,026 | 0.0 |
| R | 3 | 28 | 2877,422 | -0,025 | 0,0 | R | 3 | 27 | 2876,902 | 0,025 | 0.1 |
| R | 3 | 26 | 2876,368 | 0,029 | 0,0 | R | 3 | 25 | 2875,774 | 0,018 | 0.0 |
| R | 3 | 24 | 2875,193 | 0,002 | 0,3 | R | 3 | 23 | 2874,619 | 0,026 | 0.1 |
| R | 3 | 22 | 2874,011 | 0,008 | 0,1 | R | 3 | 21 | 2873,406 | 0,018 | 1.0 |
| R | 3 | 20 | 2872.788 | 0,013 | 0,0 | R | 3 | 19 | 2872,154 | 0,011 | 1.0 |
| R | 3 | 18 | 2871.538 | 0,030 | 0,0 | R | 3 | 17 | 2870,866 | 0,009 | 0.5 |
| R | 3 | 16 | 2870.212 | 0,013 | 0,0 | R | 3 | 15 | 2869,535 | 0,006 | 0.3 |
| R | 3 | 14 | 2868,857 | 0,006 | 0,1 | R | 3 | 13 | 2868,179 | 0,019 | 0.0 |
| R | 3 | 12 | 2867,460 | -0,001 | 0,1 | R | 3 | 11 | 2866,756 | 0,005 | 0.1 |
| R | 3 | 10 | 2866.019 | -0,012 | 0,0 | R | 3 | 9 | 2865,283 | -0,017 | 0.0 |
| R | 3 | 8 | 2864.566 | 0,006 | 0,0 | R | 3 | 7 | 2863,802 | -0,007 | 0.0 |
| R | 3 | 6 | 2863.034 | -0,014 | 0,0 | R | 3 | 5 | 2862,278 | 0,002 | 0.0 |
| R | 3 | 4 | 2861.482 | -0,012 | 0,0 | R | 3 | 3 | 2860,713 | 0,011 | 0.0 |
| R | 4 | 38 | 2881,256 | -0,034 | 0,2 | R | 4 | 37 | 2880,811 | -0,029 | 0.7 |
| R | 4 | 36 | 2880.363 | -0,028 | 0,7 | R | 4 | 35 | 2879,914 | -0,010 | 0.0 |
| R | 4 | 34 | 2879,421 | -0,031 | 0,0 | R | 4 | 33 | 2878,937 | -0.029 | 0.5 |
| R | 4 | 32 | 2878.441 | -0,033 | 0,7 | R | 4 | 31 | 2877,937 | -0.031 | 0.1 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| R | 4 | 30 | 2877.422 | -0,032 | 0.0 | R | 4 | 29 | 2876,902 | -0,025 | 0.1 |
| R | 4 | 28 | 2876.368 | -0,026 | 0.0 | R | 4 | 27 | 2875,828 | -0,019 | 0.0 |
| R | 4 | 26 | 2875.260 | -0,032 | 0.0 | R | 4 | 25 | 2874,709 | -0,016 | 1.0 |
| R | 4 | 24 | 2874.150 | 0,000 | 0.0 | R | 4 | 23 | 2873,557 | -0,006 | 0.0 |
| R | 4 | 22 | 2872.951 | -0,016 | 0.0 | R | 4 | 21 | 2872,345 | -0,014 | 0.0 |
| R | 4 | 20 | 2871.727 | -0,015 | 0.0 | R | 4 | 19 | 2871,119 | 0,004 | 0.0 |
| R | 4 | 18 | 2870.473 | -0,004 | 0.0 | R | 4 | 17 | 2869,826 | -0,003 | 0.7 |
| R | 4 | 16 | 2869.167 | -0,004 | 1.0 | R | 4 | 15 | 2868,502 | -0,000 | 0.5 |
| R | 4 | 14 | 2867.821 | -0,002 | 0.5 | R | 4 | 13 | 2867,144 | 0,010 | 0.5 |
| R | 4 | 12 | 2866.435 | 0,001 | 0.5 | R | 4 | 11 | 2865,733 | 0,008 | 0.7 |
| R | 4 | 10 | 2865.023 | 0,019 | 0.3 | R | 4 | 9 | 2864,276 | 0,002 | 0.0 |
| R | 4 | 8 | 2863.531 | -0,002 | 0.1 | R | 4 | 7 | 2862,800 | 0,018 | 0.1 |
| R | 4 | 6 | 2862.045 | 0,025 | 0.3 | R | 4 | 5 | 2861,276 | 0,026 | 0.0 |
| R | 4 | 4 | 2860.491 | 0,024 | 0.0 | R | 5 | 35 | 2878,724 | 0,040 | 0.1 |
| R | 5 | 34 | 2878.244 | 0,033 | 0.5 | R | 5 | 33 | 2877,754 | 0,027 | 0.0 |
| R | 5 | 32 | 2877.224 | -0,011 | 0.0 | R | 5 | 31 | 2876,756 | 0,026 | 0.2 |
| R | 5 | 30 | 2876.239 | 0,023 | 0.0 | R | 5 | 29 | 2875,709 | 0,017 | 0.0 |
| R | 5 | 28 | 2875.193 | 0,035 | 0.0 | R | 5 | 27 | 2874,619 | 0,006 | 0.0 |
| R | 5 | 26 | 2874.067 | 0,009 | 0.0 | R | 5 | 25 | 2873,490 | -0,002 | 0.0 |
| R | 5 | 24 | 2872.880 | -0,037 | 0.0 | R | 5 | 23 | 2872,345 | 0,014 | 0.0 |
| R | 5 | 22 | 2871.727 | -0,007 | 0.0 | R | 5 | 21 | 2871,119 | -0,009 | 0.0 |
| R | 5 | 20 | 2870.512 | 0,002 | 0.0 | R | 5 | 19 | 2869,890 | 0,006 | 0.5 |
| R | 5 | 18 | 2869.248 | 0,002 | 0.7 | R | 5 | 17 | 2868,598 | 0,000 | 0.3 |
| R | 5 | 16 | 2867.939 | -0,001 | 0.7 | R | 5 | 15 | 2867,295 | 0,024 | 0.0 |
| R | 5 | 14 | 2866.581 | -0,011 | 0.5 | R | 5 | 13 | 2865,896 | -0,006 | 0.3 |
| R | 5 | 12 | 2865.188 | -0,015 | 0.0 | R | 5 | 11 | 2864,523 | 0,030 | 0.0 |
| R | 5 | 10 | 2863.766 | -0,007 | 0.0 | R | 5 | 9 | 2863,034 | -0,008 | 0.0 |
| R | 5 | 8 | 2862.282 | -0,019 | 0.0 | R | 5 | 7 | 2861,554 | 0,004 | 0.0 |
| R | 5 | 6 | 2860.777 | -0,012 | 0.0 | R | 5 | 5 | 2860,012 | -0,005 | 0.0 |

# FREQUENCIES FOR THE (2,0,1) BAND OF 15NO2

| | K | N | OBS | O-C | WT | | K | N | OBS | O-C | WT |
|---|---|---|---|---|---|---|---|---|---|---|---|
| P | 0 | 48 | 4062.833 | -0.008 | 0.5 | P | 0 | 46 | 4065.939 | -0.015 | 0.0 |
| P | 0 | 44 | 4069.007 | 0.005 | 0.0 | P | 0 | 42 | 4071.972 | -0.016 | 0.0 |
| P | 0 | 40 | 4074.893 | -0.016 | 0.0 | P | 0 | 38 | 4077.760 | -0.008 | 0.3 |
| P | 0 | 36 | 4080.552 | -0.009 | 1.0 | P | 0 | 34 | 4083.284 | -0.008 | 1.0 |
| P | 0 | 32 | 4085.949 | -0.010 | 1.0 | P | 0 | 30 | 4088.558 | -0.006 | 1.0 |
| P | 0 | 28 | 4091.100 | -0.005 | 0.5 | P | 0 | 26 | 4093.585 | -0.001 | 1.0 |
| P | 0 | 24 | 4096.001 | -0.004 | 1.0 | P | 0 | 22 | 4098.357 | -0.006 | 0.2 |
| P | 0 | 20 | 4100.658 | -0.003 | 1.0 | P | 0 | 18 | 4102.900 | 0.000 | 0.0 |
| P | 0 | 16 | 4105.078 | -0.000 | 0.0 | P | 0 | 14 | 4107.196 | -0.001 | 0.0 |
| P | 0 | 12 | 4109.257 | 0.000 | 1.0 | P | 0 | 10 | 4111.261 | 0.003 | 1.0 |
| P | 0 | 8 | 4113.201 | 0.002 | 0.5 | P | 0 | 6 | 4115.083 | 0.002 | 1.0 |
| P | 0 | 4 | 4116.913 | 0.010 | 0.0 | P | 0 | 2 | 4118.686 | 0.020 | 0.0 |
| P | 1 | 48 | 4062.592 | -0.012 | 0.2 | P | 1 | 47 | 4064.395 | 0.008 | 0.1 |
| P | 1 | 46 | 4065.683 | -0.010 | 0.7 | P | 1 | 45 | 4067.470 | 0.000 | 0.5 |
| P | 1 | 44 | 4068.712 | -0.010 | 1.0 | P | 1 | 43 | 4070.495 | 0.006 | 0.0 |
| P | 1 | 42 | 4071.677 | -0.011 | 1.0 | P | 1 | 41 | 4073.435 | -0.011 | 0.0 |
| P | 1 | 40 | 4074.590 | -0.003 | 0.0 | P | 1 | 39 | 4076.338 | -0.001 | 1.0 |
| P | 1 | 38 | 4077.430 | -0.008 | 0.0 | P | 1 | 37 | 4079.167 | -0.003 | 0.5 |
| P | 1 | 36 | 4080.215 | -0.009 | 1.0 | P | 1 | 35 | 4081.938 | -0.000 | 1.0 |
| P | 1 | 34 | 4082.947 | -0.003 | 0.0 | P | 1 | 33 | 4084.639 | -0.004 | 1.0 |
| P | 1 | 32 | 4085.608 | -0.008 | 1.0 | P | 1 | 31 | 4087.283 | -0.002 | 1.0 |
| P | 1 | 30 | 4088.219 | -0.003 | 1.0 | P | 1 | 29 | 4089.864 | -0.001 | 1.0 |
| P | 1 | 28 | 4090.766 | -0.004 | 1.0 | P | 1 | 27 | 4092.381 | -0.002 | 1.0 |
| P | 1 | 26 | 4093.257 | -0.002 | 1.0 | P | 1 | 25 | 4094.837 | -0.001 | 1.0 |
| P | 1 | 24 | 4095.691 | 0.001 | 0.2 | P | 1 | 23 | 4097.230 | -0.001 | 0.0 |
| P | 1 | 22 | 4098.064 | 0.002 | 0.0 | P | 1 | 21 | 4099.567 | 0.006 | 0.0 |
| P | 1 | 20 | 4100.376 | 0.001 | 0.0 | P | 1 | 19 | 4101.825 | -0.005 | 0.0 |
| P | 1 | 18 | 4102.624 | -0.006 | 0.0 | P | 1 | 17 | 4104.042 | 0.006 | 0.0 |
| P | 1 | 16 | 4104.826 | -0.001 | 1.0 | P | 1 | 15 | 4106.178 | -0.003 | 0.0 |
| P | 1 | 14 | 4106.962 | -0.003 | 0.2 | P | 1 | 13 | 4108.263 | -0.000 | 1.0 |
| P | 1 | 12 | 4109.046 | 0.002 | 0.0 | P | 1 | 11 | 4110.283 | -0.001 | 0.2 |
| P | 1 | 10 | 4111.066 | 0.002 | 0.0 | P | 1 | 9 | 4112.243 | 0.001 | 0.5 |
| P | 1 | 8 | 4113.027 | 0.000 | 0.0 | P | 1 | 7 | 4114.138 | 0.000 | 0.0 |
| P | 1 | 6 | 4114.933 | 0.003 | 0.5 | P | 1 | 5 | 4115.970 | -0.002 | 1.0 |
| P | 1 | 4 | 4116.776 | 0.002 | 0.2 | P | 1 | 3 | 4117.748 | 0.005 | 0.3 |
| P | 1 | 2 | 4118.558 | -0.000 | 0.0 | P | 2 | 48 | 4062.398 | 0.002 | 0.3 |
| P | 2 | 47 | 4064.051 | 0.040 | 0.5 | P | 2 | 46 | 4065.477 | 0.001 | 0.7 |
| P | 2 | 45 | 4067.113 | 0.034 | 0.7 | P | 2 | 44 | 4068.499 | 0.002 | 1.0 |
| P | 2 | 43 | 4070.108 | 0.023 | 0.0 | P | 2 | 42 | 4071.464 | 0.003 | 1.0 |
| P | 2 | 41 | 4073.064 | 0.033 | 1.0 | P | 2 | 40 | 4074.373 | 0.006 | 1.0 |
| P | 2 | 39 | 4075.951 | 0.036 | 0.7 | P | 2 | 38 | 4077.223 | 0.007 | 1.0 |
| P | 2 | 37 | 4078.757 | 0.020 | 0.0 | P | 2 | 36 | 4080.014 | 0.007 | 1.0 |
| P | 2 | 35 | 4081.514 | 0.015 | 0.0 | P | 2 | 34 | 4082.752 | 0.012 | 0.0 |
| P | 2 | 33 | 4084.214 | 0.013 | 0.0 | P | 2 | 32 | 4085.422 | 0.007 | 0.0 |
| P | 2 | 31 | 4086.852 | 0.011 | 1.0 | P | 2 | 30 | 4088.040 | 0.006 | 0.1 |
| P | 2 | 29 | 4089.433 | 0.011 | 1.0 | P | 2 | 28 | 4090.603 | 0.011 | 1.0 |
| P | 2 | 27 | 4091.949 | 0.008 | 1.0 | P | 2 | 26 | 4093.096 | 0.004 | 1.0 |
| P | 2 | 25 | 4094.402 | 0.003 | 1.0 | P | 2 | 24 | 4095.538 | 0.006 | 1.0 |
| P | 2 | 23 | 4096.804 | 0.006 | 0.5 | P | 2 | 22 | 4097.918 | 0.006 | 1.0 |
| P | 2 | 21 | 4099.143 | 0.007 | 1.0 | P | 2 | 20 | 4100.237 | 0.005 | 1.0 |

```
P  2 19 4101.418   0,005 1.0      P  2 18 4102,494   0,004 0.5
P  2 17 4103.637   0,006 0.3      P  2 16 4104,690   0,003 1.0
P  2 15 4105.802   0,015 0.0      P  2 14 4106,836   0,014 0.0
P  2 13 4107.885   0,001 0.0      P  2 12 4108,896   0,001 0.0
P  2 11 4109.913  -0,006 0.0      P  2 10 4110,901  -0,005 0.0
P  2  9 4111.897   0,002 0.0      P  2  8 4112,855   0,000 0.0
P  2  7 4113.810   0,000 0.0      P  2  6 4114,740  -0,002 0.0
P  2  5 4115.666   0,002 1.0      P  2  4 4116,579   0,012 0.1
P  2  3 4117.462   0,004 0.5      P  3 48 4061,873  -0,140 0.0
P  3 47 4063.477  -0,091 0.0      P  3 46 4064,965  -0,133 0.0
P  3 45 4066.537  -0,092 0.0      P  3 44 4068,007  -0,119 0.0
P  3 43 4069.534  -0,097 0.0      P  3 42 4070,980  -0,116 0.0
P  3 41 4072.484  -0,089 0.0      P  3 40 4073,900  -0,108 0.0
P  3 39 4075.363  -0,092 0.0      P  3 38 4076,757  -0,103 0.0
P  3 37 4078.186  -0,091 0.0      P  3 36 4079,557  -0,097 0.0
P  3 35 4080.949  -0,091 0.0      P  3 34 4082,294  -0,094 0.0
P  3 33 4083.660  -0,082 0.0      P  3 32 4084,975  -0,087 0.0
P  3 31 4086.311  -0,075 0.0      P  3 30 4087,601  -0,075 0.0
P  3 29 4088.884  -0,084 0.0      P  3 28 4090,146  -0,085 0.0
P  3 27 4091.418  -0,072 0.0      P  3 26 4092,656  -0,068 0.0
P  3 25 4093.884  -0,066 0.0      P  3 24 4095,096  -0,061 0.0
P  3 23 4096.297  -0,057 0.0      P  3 22 4097,478  -0,052 0.0
P  3 21 4098.638  -0,058 0.0      P  3 20 4099,792  -0,050 0.0
P  3 19 4100.928  -0,048 0.0      P  3 18 4102,054  -0,039 0.0
P  3 17 4103.157  -0,039 0.0      P  3 16 4104,250  -0,034 0.0
P  3 15 4105.324  -0,030 0.0      P  3 14 4106,384  -0,029 0.0
P  3 13 4107.431  -0,024 0.0      P  3 12 4108,460  -0,021 0.0
P  3 11 4109.476  -0,017 0.0      P  3 10 4110,472  -0,017 0.3
P  3  9 4111.460  -0,010 0.7      P  3  8 4112,424  -0,011 0.2
P  3  7 4113.382  -0,004 0.3      P  3  6 4114,316  -0,005 1.0
P  3  5 4115.237  -0,004 0.5      P  3  4 4116,137  -0,009 1.0
P  4 48 4061.385  -0,048 0.0      P  4 47 4062,952  -0,032 0.0
P  4 46 4064.486  -0,035 0.3      P  4 45 4066,011  -0,033 0.5
P  4 44 4067.521  -0,030 0.5      P  4 43 4069,007  -0,036 0.0
P  4 42 4070.495  -0,026 0.0      P  4 41 4071,972  -0,012 0.0
P  4 40 4073.435   0,003 0.0      P  4 39 4074,860  -0,006 0.1
P  4 38 4076.278  -0,005 1.0      P  4 37 4077,674  -0,013 0.2
P  4 36 4079.064  -0,011 0.2      P  4 35 4080,440  -0,009 1.0
P  4 34 4081.801  -0,006 1.0      P  4 33 4083,144  -0,006 1.0
P  4 32 4084.474  -0,005 1.0      P  4 31 4085,787  -0,006 1.0
P  4 30 4087.085  -0,005 1.0      P  4 29 4088,369  -0,005 1.0
P  4 28 4089.640  -0,002 1.0      P  4 27 4090,891  -0,005 1.0
P  4 26 4092.132  -0,002 1.0      P  4 25 4093,358   0,001 0.5
P  4 24 4094.563  -0,002 1.0      P  4 23 4095,758  -0,000 0.5
P  4 22 4096.935  -0,001 1.0      P  4 21 4098,093  -0,005 0.0
P  4 20 4099.249   0,003 1.0      P  4 19 4100,376  -0,003 0.0
P  4 18 4101.497   0,000 0.3      P  4 17 4102,596  -0,002 0.0
P  4 16 4103.685  -0,001 0.2      P  4 15 4104,757  -0,000 1.0
P  4 14 4105.802  -0,012 0.0      P  4 13 4106,836  -0,020 0.0
P  4 12 4107.885   0,003 0.0      P  4 11 4108,896   0,003 0.0
P  4 10 4109.880  -0,009 0.0      P  4  9 4110,868  -0,003 0.0
P  4  8 4111.837   0,001 0.0      P  4  7 4112,787   0,001 0.2
P  4  6 4113.724   0,005 0.0      P  4  5 4114,634  -0,008 0.5
P  5 48 4060.700   0,005 0.1      P  5 47 4062,249   0,004 0.1
```

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| P | 5 | 46 | 4063,793 | 0,013 | 0,1 | P | 5 | 45 | 4065,304 | 0,003 | 0,3 |
| P | 5 | 44 | 4066,813 | 0,006 | 0,1 | P | 5 | 43 | 4068,300 | 0,003 | 1,0 |
| P | 5 | 42 | 4069,771 | -0,003 | 1,0 | P | 5 | 41 | 4071,244 | 0,009 | 1,0 |
| P | 5 | 40 | 4072,684 | 0,003 | 1,0 | P | 5 | 39 | 4074,122 | 0,009 | 0,3 |
| P | 5 | 38 | 4075,538 | 0,009 | 1,0 | P | 5 | 37 | 4076,937 | 0,006 | 1,0 |
| P | 5 | 36 | 4078,324 | 0,008 | 0,7 | P | 5 | 35 | 4079,696 | 0,006 | 1,0 |
| P | 5 | 34 | 4081,048 | 0,002 | 1,0 | P | 5 | 33 | 4082,391 | 0,002 | 0,7 |
| P | 5 | 32 | 4083,717 | 0,002 | 1,0 | P | 5 | 31 | 4085,030 | 0,003 | 1,0 |
| P | 5 | 30 | 4086,311 | -0,013 | 0,0 | P | 5 | 29 | 4087,601 | -0,005 | 0,0 |
| P | 5 | 28 | 4088,884 | 0,011 | 0,0 | P | 5 | 27 | 4090,119 | -0,006 | 0,0 |
| P | 5 | 26 | 4091,368 | 0,006 | 0,7 | P | 5 | 25 | 4092,587 | 0,003 | 1,0 |
| P | 5 | 24 | 4093,793 | 0,002 | 0,5 | P | 5 | 23 | 4094,984 | 0,001 | 1,0 |
| P | 5 | 22 | 4096,161 | 0,001 | 1,0 | P | 5 | 21 | 4097,326 | 0,005 | 1,0 |
| P | 5 | 20 | 4098,468 | -0,000 | 1,0 | P | 5 | 19 | 4099,600 | 0,000 | 0,0 |
| P | 5 | 18 | 4100,714 | -0,001 | 0,1 | P | 5 | 17 | 4101,825 | 0,007 | 0,0 |
| P | 5 | 16 | 4102,898 | -0,006 | 0,0 | P | 5 | 15 | 4103,979 | 0,003 | 0,3 |
| P | 5 | 14 | 4105,038 | 0,006 | 0,0 | P | 5 | 13 | 4106,075 | 0,002 | 0,1 |
| P | 5 | 12 | 4107,102 | 0,003 | 0,1 | P | 5 | 11 | 4108,114 | 0,004 | 1,0 |
| P | 5 | 10 | 4109,105 | -0,001 | 0,0 | P | 5 | 9 | 4110,084 | -0,002 | 0,5 |
| P | 5 | 8 | 4111,055 | 0,003 | 0,0 | P | 5 | 7 | 4111,993 | -0,009 | 0,0 |
| P | 5 | 6 | 4112,953 | 0,016 | 0,0 | P | 6 | 47 | 4061,358 | -0,001 | 0,0 |
| P | 6 | 46 | 4062,889 | -0,001 | 0,1 | P | 6 | 45 | 4064,395 | -0,012 | 0,0 |
| P | 6 | 44 | 4065,904 | -0,004 | 0,0 | P | 6 | 43 | 4067,400 | 0,004 | 0,3 |
| P | 6 | 42 | 4068,866 | -0,002 | 0,3 | P | 6 | 41 | 4070,328 | 0,002 | 0,5 |
| P | 6 | 40 | 4071,771 | 0,002 | 0,5 | P | 6 | 39 | 4073,200 | 0,004 | 1,0 |
| P | 6 | 38 | 4074,614 | 0,005 | 0,0 | P | 6 | 37 | 4076,007 | -0,001 | 0,1 |
| P | 6 | 36 | 4077,397 | 0,006 | 0,0 | P | 6 | 35 | 4078,757 | -0,003 | 0,0 |
| P | 6 | 34 | 4080,114 | 0,001 | 1,0 | P | 6 | 33 | 4081,457 | 0,005 | 0,3 |
| P | 6 | 32 | 4082,773 | -0,004 | 0,0 | P | 6 | 31 | 4084,086 | 0,000 | 0,1 |
| P | 6 | 30 | 4085,384 | 0,004 | 0,0 | P | 6 | 29 | 4086,663 | 0,003 | 1,0 |
| P | 6 | 28 | 4087,927 | 0,004 | 0,1 | P | 6 | 27 | 4089,171 | -0,002 | 0,0 |
| P | 6 | 26 | 4090,408 | -0,000 | 1,0 | P | 6 | 25 | 4091,627 | -0,001 | 1,0 |
| P | 6 | 24 | 4092,835 | 0,002 | 0,0 | P | 6 | 23 | 4094,028 | 0,006 | 0,0 |
| P | 6 | 22 | 4095,199 | 0,001 | 0,1 | P | 6 | 21 | 4096,347 | -0,010 | 0,0 |
| P | 6 | 20 | 4097,502 | -0,000 | 0,0 | P | 6 | 19 | 4098,638 | 0,005 | 0,0 |
| P | 6 | 18 | 4099,752 | 0,004 | 0,1 | P | 6 | 17 | 4100,844 | -0,004 | 0,3 |
| P | 6 | 16 | 4101,934 | 0,001 | 0,5 | P | 6 | 15 | 4102,999 | -0,004 | 0,5 |
| P | 6 | 14 | 4104,042 | -0,016 | 0,0 | P | 6 | 13 | 4105,078 | -0,020 | 0,0 |
| P | 6 | 12 | 4106,108 | -0,015 | 0,0 | P | 6 | 11 | 4107,130 | -0,003 | 0,0 |
| P | 6 | 10 | 4108,112 | -0,016 | 0,0 | P | 6 | 9 | 4109,105 | -0,004 | 0,0 |
| P | 6 | 8 | 4110,068 | -0,005 | 0,0 | P | 6 | 7 | 4111,016 | -0,007 | 0,0 |
| P | 7 | 45 | 4063,364 | -0,008 | 0,0 | P | 7 | 44 | 4064,861 | -0,005 | 0,0 |
| P | 7 | 43 | 4066,336 | -0,010 | 0,0 | P | 7 | 42 | 4067,804 | -0,008 | 0,1 |
| P | 7 | 41 | 4069,253 | -0,010 | 0,1 | P | 7 | 40 | 4070,689 | -0,010 | 0,1 |
| P | 7 | 39 | 4072,126 | 0,005 | 0,0 | P | 7 | 38 | 4073,523 | -0,006 | 0,1 |
| P | 7 | 37 | 4074,893 | -0,027 | 0,0 | P | 7 | 36 | 4076,278 | -0,020 | 0,0 |
| P | 7 | 35 | 4077,674 | 0,013 | 0,0 | P | 7 | 34 | 4079,007 | -0,003 | 0,2 |
| P | 7 | 33 | 4080,342 | -0,001 | 0,2 | P | 7 | 32 | 4081,665 | 0,003 | 0,0 |
| P | 7 | 31 | 4082,947 | -0,020 | 0,0 | P | 7 | 30 | 4084,249 | -0,007 | 0,0 |
| P | 7 | 29 | 4085,524 | -0,007 | 1,0 | P | 7 | 28 | 4086,788 | -0,003 | 1,0 |
| P | 7 | 27 | 4088,040 | 0,003 | 0,0 | P | 7 | 26 | 4089,265 | -0,002 | 1,0 |
| P | 7 | 25 | 4090,481 | -0,002 | 1,0 | P | 7 | 24 | 4091,677 | -0,007 | 1,0 |
| P | 7 | 23 | 4092,859 | -0,012 | 0,0 | P | 7 | 22 | 4094,028 | -0,014 | 0,0 |
| P | 7 | 21 | 4095,199 | -0,000 | 0,0 | P | 7 | 20 | 4096,347 | 0,007 | 0,0 |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| P | 7 | 19 | 4097.478 | 0,010 | 0.0 | P | 7 | 18 | 4098,581 | 0,001 | 0.1 |
| P | 7 | 17 | 4099.677 | -0,001 | 1.0 | P | 7 | 16 | 4100,755 | -0,006 | 0.0 |
| P | 7 | 15 | 4101.825 | -0,004 | 0.0 | P | 7 | 14 | 4102,900 | 0,018 | 0.0 |
| P | 7 | 13 | 4103.918 | -0,002 | 0.0 | P | 7 | 12 | 4104,938 | -0,006 | 0.2 |
| P | 7 | 11 | 4105.950 | -0,003 | 0.2 | P | 7 | 10 | 4106,936 | -0,010 | 0.0 |
| P | 7 | 9 | 4107.932 | 0,007 | 0.0 | P | 7 | 8 | 4108,889 | -0,000 | 0.0 |
| P | 8 | 40 | 4069.491 | 0,010 | 0.0 | P | 8 | 39 | 4070,896 | 0,003 | 0.1 |
| P | 8 | 38 | 4072.300 | 0,011 | 0.0 | P | 8 | 37 | 4073,681 | 0,008 | 0.1 |
| P | 8 | 36 | 4075.038 | -0,004 | 0.1 | P | 8 | 35 | 4076,391 | -0,005 | 0.1 |
| P | 8 | 34 | 4077.760 | 0,024 | 0.0 | P | 8 | 33 | 4079,064 | 0,004 | 0.0 |
| P | 8 | 32 | 4080.381 | 0,009 | 0.1 | P | 8 | 31 | 4081,665 | -0,003 | 0.1 |
| P | 8 | 30 | 4082.947 | -0,003 | 0.0 | P | 8 | 29 | 4084,214 | -0,004 | 0.0 |
| P | 8 | 28 | 4085.461 | -0,010 | 0.0 | P | 8 | 27 | 4086,711 | 0,002 | 0.5 |
| P | 8 | 26 | 4087.927 | -0,006 | 0.0 | P | 8 | 25 | 4089,171 | 0,028 | 0.0 |
| P | 8 | 24 | 4090.344 | 0,005 | 1.0 | P | 8 | 23 | 4091,518 | -0,002 | 1.0 |
| P | 8 | 22 | 4092.690 | 0,004 | 0.0 | P | 8 | 21 | 4093,845 | 0,008 | 0.0 |
| P | 8 | 20 | 4094.984 | 0,010 | 0.0 | P | 8 | 19 | 4096,105 | 0,009 | 0.3 |
| P | 8 | 18 | 4097.230 | 0,025 | 0.0 | P | 8 | 17 | 4098,307 | 0,008 | 0.0 |
| P | 8 | 16 | 4099.383 | 0,006 | 0.5 | P | 8 | 15 | 4100,415 | -0,027 | 0.0 |
| P | 8 | 14 | 4101.497 | 0,005 | 0.0 | P | 8 | 13 | 4102,494 | -0,034 | 0.0 |
| P | 8 | 12 | 4103.560 | 0,012 | 0.0 | P | 8 | 11 | 4104,573 | 0,019 | 0.0 |
| P | 8 | 10 | 4105.544 | -0,002 | 0.0 | P | 8 | 9 | 4106,511 | -0,012 | 0.0 |
| Q | 1 | 1 | 4120.295 | 0,002 | 0.7 | Q | 1 | 2 | 4120,168 | 0,004 | 0.7 |
| Q | 1 | 3 | 4120.343 | 0,002 | 0.1 | Q | 1 | 5 | 4120,423 | -0,002 | 0.5 |
| Q | 1 | 7 | 4120.552 | 0,005 | 0.1 | Q | 1 | 9 | 4120,704 | -0,004 | 0.1 |
| Q | 2 | 2 | 4119.987 | 0,000 | 0.5 | Q | 2 | 3 | 4119,943 | 0,001 | 0.5 |
| Q | 2 | 4 | 4119.881 | 0,001 | 1.0 | Q | 2 | 5 | 4119,806 | -0,001 | 1.0 |
| Q | 2 | 6 | 4119.707 | -0,001 | 1.0 | Q | 2 | 7 | 4119,614 | 0,000 | 0.3 |
| Q | 3 | 3 | 4119.519 | -0,001 | 1.0 | Q | 3 | 4 | 4119,460 | 0,001 | 1.0 |
| Q | 3 | 5 | 4119.377 | -0,005 | 1.0 | Q | 3 | 6 | 4119,286 | -0,005 | 1.0 |
| Q | 3 | 7 | 4119.172 | -0,012 | 1.0 | Q | 3 | 8 | 4119,056 | -0,006 | 0.3 |
| Q | 3 | 9 | 4118.908 | -0,017 | 0.1 | Q | 3 | 10 | 4118,765 | -0,007 | 0.0 |
| Q | 4 | 4 | 4118.864 | 0,004 | 0.5 | Q | 4 | 5 | 4118,786 | 0,002 | 0.1 |
| Q | 4 | 6 | 4118.686 | -0,007 | 0.0 | Q | 4 | 7 | 4118,583 | -0,003 | 0.1 |
| Q | 4 | 8 | 4118.464 | 0,000 | 1.0 | Q | 4 | 9 | 4118,326 | -0,001 | 0.7 |
| Q | 4 | 10 | 4118.182 | 0,007 | 0.5 | Q | 4 | 11 | 4118,002 | -0,005 | 0.0 |
| Q | 5 | 5 | 4118.002 | 0,001 | 0.1 | Q | 5 | 6 | 4117,911 | 0,001 | 0.5 |
| Q | 5 | 7 | 4117.809 | 0,005 | 0.5 | Q | 5 | 8 | 4117,685 | 0,002 | 0.5 |
| Q | 5 | 9 | 4117.544 | -0,001 | 0.7 | Q | 5 | 10 | 4117,398 | 0,004 | 0.1 |
| Q | 5 | 11 | 4117.229 | 0,002 | 0.3 | Q | 5 | 12 | 4117,049 | 0,004 | 1.0 |
| Q | 5 | 13 | 4116.834 | -0,013 | 0.1 | Q | 5 | 14 | 4116,632 | -0,003 | 0.1 |
| Q | 5 | 15 | 4116.415 | 0,008 | 0.0 | Q | 6 | 6 | 4116,939 | 0,004 | 0.0 |
| Q | 6 | 7 | 4116.834 | 0,006 | 0.1 | Q | 6 | 8 | 4116,703 | -0,005 | 0.5 |
| Q | 6 | 9 | 4116.574 | 0,002 | 0.0 | Q | 6 | 10 | 4116,415 | -0,007 | 0.1 |
| Q | 6 | 11 | 4116.256 | 0,001 | 0.5 | Q | 6 | 12 | 4116,073 | -0,002 | 0.1 |
| Q | 6 | 13 | 4115.883 | 0,005 | 0.0 | Q | 6 | 14 | 4115,663 | -0,004 | 0.0 |
| Q | 6 | 15 | 4115.435 | -0,006 | 0.1 | Q | 7 | 7 | 4115,663 | 0,014 | 0.0 |
| Q | 7 | 8 | 4115.525 | -0,004 | 0.3 | Q | 7 | 9 | 4115,390 | -0,005 | 0.1 |
| Q | 7 | 10 | 4115.252 | 0,006 | 0.0 | Q | 7 | 11 | 4115,083 | 0,001 | 0.0 |
| Q | 7 | 12 | 4114.933 | 0,030 | 0.0 | Q | 7 | 13 | 4114,743 | 0,034 | 0.0 |
| Q | 7 | 14 | 4114.498 | -0,002 | 0.7 | Q | 7 | 15 | 4114,293 | 0,017 | 0.0 |
| Q | 8 | 8 | 4114.138 | 0,007 | 0.0 | Q | 8 | 9 | 4114,027 | 0,027 | 0.0 |
| Q | 8 | 11 | 4113.684 | -0,008 | 0.0 | Q | 8 | 12 | 4113,513 | -0,004 | 0.5 |
| Q | 8 | 14 | 4113.134 | 0,013 | 0.0 | R | 0 | 46 | 4141,363 | 0,008 | 0.0 |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| R | 0 | 44 | 4141.217 | -0.010 | 0.0 | R | 0 | 42 | 4141,010 | -0.023 | 0.0 |
| R | 0 | 40 | 4140.741 | -0.032 | 0.2 | R | 0 | 38 | 4140,443 | -0.002 | 0.2 |
| R | 0 | 36 | 4140.042 | -0.009 | 0.0 | R | 0 | 34 | 4139,571 | -0.017 | 0.0 |
| R | 0 | 32 | 4139.037 | -0.020 | 0.0 | R | 0 | 30 | 4138,461 | 0,005 | 0.0 |
| R | 0 | 28 | 4137.793 | 0,006 | 0.0 | R | 0 | 26 | 4137,046 | 0,001 | 0.1 |
| R | 0 | 24 | 4136.229 | -0,006 | 1.0 | R | 0 | 22 | 4135,350 | -0,004 | 1.0 |
| R | 0 | 20 | 4134.395 | -0,007 | 0.3 | R | 0 | 18 | 4133,380 | -0,001 | 1.0 |
| R | 0 | 16 | 4132.291 | -0,000 | 0.5 | R | 0 | 14 | 4131,132 | -0,001 | 1.0 |
| R | 0 | 12 | 4129.902 | -0,006 | 0.1 | R | 0 | 10 | 4128,611 | -0,005 | 0.0 |
| R | 0 | 8 | 4127.265 | 0,005 | 0.0 | R | 0 | 6 | 4125,845 | 0,007 | 0.0 |
| R | 0 | 4 | 4124.345 | -0,008 | 0.0 | R | 0 | 2 | 4122,797 | -0,008 | 0.0 |
| R | 0 | 0 | 4121.195 | -0,000 | 1.0 | R | 1 | 47 | 4141,217 | -0,025 | 0.0 |
| R | 1 | 46 | 4142.888 | 0,002 | 0.1 | R | 1 | 45 | 4141,126 | 0,010 | 0.0 |
| R | 1 | 44 | 4142.674 | -0,006 | 0.5 | R | 1 | 43 | 4140,936 | 0,002 | 0.2 |
| R | 1 | 42 | 4142.397 | -0,004 | 0.5 | R | 1 | 41 | 4140,681 | -0,005 | 0.1 |
| R | 1 | 40 | 4142.040 | -0,009 | 0.5 | R | 1 | 39 | 4140,373 | 0,001 | 0.2 |
| R | 1 | 38 | 4141.621 | -0,006 | 0.3 | R | 1 | 37 | 4139,997 | 0,007 | 0.0 |
| R | 1 | 36 | 4141.126 | -0,008 | 0.0 | R | 1 | 35 | 4139,535 | -0,007 | 0.0 |
| R | 1 | 34 | 4140.561 | -0,010 | 0.2 | R | 1 | 33 | 4139,037 | 0,010 | 0.0 |
| R | 1 | 32 | 4139.932 | -0,008 | 0.5 | R | 1 | 31 | 4138,461 | 0,014 | 0.0 |
| R | 1 | 30 | 4139.234 | -0,008 | 0.0 | R | 1 | 29 | 4137,788 | -0,011 | 0.0 |
| R | 1 | 28 | 4138.461 | -0,015 | 0.0 | R | 1 | 27 | 4137,083 | -0,004 | 0.1 |
| R | 1 | 26 | 4137.640 | -0,004 | 0.3 | R | 1 | 25 | 4136,313 | 0,005 | 0.0 |
| R | 1 | 24 | 4136.745 | -0,004 | 1.0 | R | 1 | 23 | 4135,463 | -0,000 | 1.0 |
| R | 1 | 22 | 4135.785 | -0,003 | 1.0 | R | 1 | 21 | 4134,551 | -0,002 | 1.0 |
| R | 1 | 20 | 4134.756 | -0,008 | 0.0 | R | 1 | 19 | 4133,576 | -0,001 | 1.0 |
| R | 1 | 18 | 4133.672 | -0,004 | 0.0 | R | 1 | 17 | 4132,532 | -0,005 | 0.0 |
| R | 1 | 16 | 4132.532 | 0,005 | 0.0 | R | 1 | 15 | 4131,435 | 0,004 | 0.0 |
| R | 1 | 14 | 4131.315 | 0,001 | 0.3 | R | 1 | 13 | 4130,253 | -0,008 | 0.0 |
| R | 1 | 12 | 4130.042 | 0,001 | 1.0 | R | 1 | 11 | 4129,033 | 0,005 | 0.1 |
| R | 1 | 10 | 4128.708 | 0,002 | 0.1 | R | 1 | 9 | 4127,735 | 0,006 | 1.0 |
| R | 1 | 8 | 4127.306 | -0,005 | 0.1 | R | 1 | 7 | 4126,366 | -0,000 | 1.0 |
| R | 1 | 6 | 4125.845 | -0,009 | 0.0 | R | 1 | 5 | 4124,940 | -0,001 | 0.3 |
| R | 1 | 4 | 4124.345 | 0,007 | 0.0 | R | 1 | 3 | 4123,451 | -0,000 | 0.3 |
| R | 1 | 2 | 4122.769 | 0,001 | 0.0 | R | 1 | 1 | 4121,903 | 0,004 | 1.0 |
| R | 2 | 47 | 4142.040 | -0,012 | 0.0 | R | 2 | 46 | 4143,240 | 0,004 | 0.1 |
| R | 2 | 45 | 4141.890 | 0,009 | 0.0 | R | 2 | 44 | 4142,911 | -0,005 | 0.1 |
| R | 2 | 43 | 4141.621 | -0,022 | 0.0 | R | 2 | 42 | 4142,538 | 0,006 | 0.0 |
| R | 2 | 41 | 4141.369 | 0,031 | 0.0 | R | 2 | 40 | 4142,087 | 0,003 | 0.5 |
| R | 2 | 39 | 4141.010 | 0,044 | 0.0 | R | 2 | 38 | 4141,577 | 0,005 | 0.5 |
| R | 2 | 37 | 4140.561 | 0,032 | 0.1 | R | 2 | 36 | 4141,010 | 0,011 | 0.0 |
| R | 2 | 35 | 4140.042 | 0,016 | 0.0 | R | 2 | 34 | 4140,373 | 0,008 | 1.0 |
| R | 2 | 33 | 4139.493 | 0,037 | 0.0 | R | 2 | 32 | 4139,676 | 0,004 | 0.2 |
| R | 2 | 31 | 4138.840 | 0,017 | 0.0 | R | 2 | 30 | 4138,926 | 0,007 | 0.0 |
| R | 2 | 29 | 4138.133 | 0,009 | 0.0 | R | 2 | 28 | 4138,133 | 0,022 | 0.0 |
| R | 2 | 27 | 4137.378 | 0,018 | 0.1 | R | 2 | 26 | 4137,245 | -0,001 | 0.0 |
| R | 2 | 25 | 4136.552 | 0,020 | 0.0 | R | 2 | 24 | 4136,313 | -0,010 | 0.0 |
| R | 2 | 23 | 4135.651 | 0,011 | 0.0 | R | 2 | 22 | 4135,350 | 0,003 | 0.1 |
| R | 2 | 21 | 4134.690 | 0,006 | 0.0 | R | 2 | 20 | 4134,324 | 0,009 | 0.1 |
| R | 2 | 19 | 4133.672 | 0,009 | 0.0 | R | 2 | 18 | 4133,224 | -0,003 | 0.0 |
| R | 2 | 17 | 4132.584 | 0,002 | 0.0 | R | 2 | 16 | 4132,091 | 0,007 | 0.3 |
| R | 2 | 15 | 4131.435 | -0,000 | 0.0 | R | 2 | 14 | 4130,893 | 0,008 | 0.3 |
| R | 2 | 13 | 4130.242 | 0,015 | 0.0 | R | 2 | 12 | 4129,637 | 0,008 | 0.0 |
| R | 2 | 11 | 4128.960 | 0,004 | 1.0 | R | 2 | 10 | 4128,318 | 0,003 | 1.0 |

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|---|---|---|---|---|---|---|---|---|---|
| R | 2 | 9 | 4127,627 | 0,004 | 1.0 | R | 2 | 8 | 4126,946 | 0,003 | 0.2 |
| R | 2 | 7 | 4126,231 | 0,002 | 1.0 | R | 2 | 6 | 4125,513 | 0,001 | 0,5 |
| R | 2 | 5 | 4124,772 | 0,000 | 0.5 | R | 2 | 4 | 4124,022 | 0,000 | 1.0 |
| R | 2 | 3 | 4123,254 | 0,000 | 1.0 | R | 2 | 2 | 4122,475 | 0,003 | 1.0 |
| R | 3 | 46 | 4142,279 | -0,051 | 0.0 | R | 3 | 45 | 4141,799 | -0,084 | 0,0 |
| R | 3 | 44 | 4141,909 | -0,103 | 0.0 | R | 3 | 43 | 4141,514 | -0,082 | 0.0 |
| R | 3 | 42 | 4141,514 | -0,126 | 0.0 | R | 3 | 41 | 4141,126 | -0,119 | 0.0 |
| R | 3 | 40 | 4141,126 | -0,086 | 0.0 | R | 3 | 39 | 4140,741 | -0,090 | 0.0 |
| R | 3 | 38 | 4140,616 | -0,113 | 0.0 | R | 3 | 37 | 4140,260 | -0,094 | 0.0 |
| R | 3 | 36 | 4140,082 | -0,108 | 0.0 | R | 3 | 35 | 4139,724 | -0,091 | 0.0 |
| R | 3 | 34 | 4139,493 | -0,102 | 0.0 | R | 3 | 33 | 4139,125 | -0,088 | 0.0 |
| R | 3 | 32 | 4138,840 | -0,104 | 0.0 | R | 3 | 31 | 4138,461 | -0,089 | 0.0 |
| R | 3 | 30 | 4138,133 | -0,101 | 0.0 | R | 3 | 29 | 4137,751 | -0,074 | 0.0 |
| R | 3 | 28 | 4137,378 | -0,089 | 0.0 | R | 3 | 27 | 4136,964 | -0,075 | 0,0 |
| R | 3 | 26 | 4136,552 | -0,089 | 0.0 | R | 3 | 25 | 4136,115 | -0,076 | 0.0 |
| R | 3 | 24 | 4135,683 | -0,073 | 0.0 | R | 3 | 23 | 4135,215 | -0,066 | 0.0 |
| R | 3 | 22 | 4134,756 | -0,056 | 0.0 | R | 3 | 21 | 4134,253 | -0,058 | 0.0 |
| R | 3 | 20 | 4133,744 | -0,063 | 0.0 | R | 3 | 19 | 4133,224 | -0,055 | 0.0 |
| R | 3 | 18 | 4132,688 | -0,055 | 0.0 | R | 3 | 17 | 4132,144 | -0,043 | 0.0 |
| R | 3 | 16 | 4131,583 | -0,036 | 0.0 | R | 3 | 15 | 4131,005 | -0,028 | 0.0 |
| R | 3 | 14 | 4130,408 | -0,027 | 0.0 | R | 3 | 13 | 4129,791 | -0,028 | 0.0 |
| R | 3 | 12 | 4129,161 | -0,028 | 0.0 | R | 3 | 11 | 4128,521 | -0,023 | 0.0 |
| R | 3 | 10 | 4127,860 | -0,023 | 0.0 | R | 3 | 9 | 4127,192 | -0,015 | 0.1 |
| R | 3 | 8 | 4126,502 | -0,014 | 0,5 | R | 3 | 7 | 4125,802 | -0,008 | 0,0 |
| R | 3 | 6 | 4125,073 | -0,016 | 0.0 | R | 3 | 5 | 4124,345 | -0,007 | 0.0 |
| R | 3 | 4 | 4123,600 | -0,000 | 0,5 | R | 3 | 3 | 4122,841 | 0,009 | 0.0 |
| R | 4 | 45 | 4141,310 | -0,030 | 0.1 | R | 4 | 44 | 4141,217 | 0,000 | 0.0 |
| R | 4 | 43 | 4141,010 | -0,030 | 0.0 | R | 4 | 42 | 4140,850 | -0,031 | 0.3 |
| R | 4 | 41 | 4140,681 | 0,002 | 0.0 | R | 4 | 40 | 4140,443 | -0,043 | 0.0 |
| R | 4 | 39 | 4140,260 | 0,002 | 0.0 | R | 4 | 38 | 4139,997 | -0,034 | 0.0 |
| R | 4 | 37 | 4139,750 | -0,025 | 0.0 | R | 4 | 36 | 4139,493 | -0,022 | 0.0 |
| R | 4 | 35 | 4139,234 | 0,003 | 0.0 | R | 4 | 34 | 4138,926 | -0,013 | 0.0 |
| R | 4 | 33 | 4138,617 | -0,010 | 1.0 | R | 4 | 32 | 4138,297 | -0,006 | 1.0 |
| R | 4 | 31 | 4137,954 | -0,005 | 1.0 | R | 4 | 30 | 4137,602 | -0,003 | 0.3 |
| R | 4 | 29 | 4137,215 | -0,019 | 0.0 | R | 4 | 28 | 4136,846 | -0,002 | 0.0 |
| R | 4 | 27 | 4136,448 | 0,002 | 0.0 | R | 4 | 26 | 4136,029 | -0,001 | 1.0 |
| R | 4 | 25 | 4135,597 | -0,000 | 0.3 | R | 4 | 24 | 4135,154 | 0,004 | 1,0 |
| R | 4 | 23 | 4134,690 | 0,002 | 0.0 | R | 4 | 22 | 4134,215 | 0,005 | 0.3 |
| R | 4 | 21 | 4133,715 | -0,002 | 0.0 | R | 4 | 20 | 4133,224 | 0,016 | 0.0 |
| R | 4 | 19 | 4132,688 | 0,003 | 0.0 | R | 4 | 18 | 4132,144 | -0,002 | 0.0 |
| R | 4 | 17 | 4131,583 | -0,009 | 0.0 | R | 4 | 16 | 4131,005 | -0,019 | 0.0 |
| R | 4 | 15 | 4130,433 | -0,006 | 0.0 | R | 4 | 14 | 4129,840 | 0,001 | 0.1 |
| R | 4 | 13 | 4129,224 | 0,000 | 0.0 | R | 4 | 12 | 4128,611 | 0,017 | 0.0 |
| R | 4 | 11 | 4127,949 | 0,000 | 0.7 | R | 4 | 10 | 4127,285 | -0,002 | 0.0 |
| R | 4 | 9 | 4126,614 | 0,003 | 0.7 | R | 4 | 8 | 4125,915 | -0,005 | 0.0 |
| R | 4 | 7 | 4125,217 | 0,003 | 0.0 | R | 4 | 6 | 4124,498 | 0,006 | 0.0 |
| R | 4 | 5 | 4123,759 | 0,004 | 0.0 | R | 4 | 4 | 4123,003 | 0,001 | 0.0 |
| R | 5 | 38 | 4139,272 | 0,001 | 0.0 | R | 5 | 37 | 4139,037 | 0,017 | 0.0 |
| R | 5 | 36 | 4138,762 | 0,006 | 0.3 | R | 5 | 35 | 4138,461 | -0,014 | 0.0 |
| R | 5 | 34 | 4138,181 | 0,001 | 0.0 | R | 5 | 33 | 4137,863 | -0,006 | 0.1 |
| R | 5 | 32 | 4137,559 | 0,015 | 0.1 | R | 5 | 31 | 4137,215 | 0,013 | 0.0 |
| R | 5 | 30 | 4136,846 | 0,000 | 0.0 | R | 5 | 29 | 4136,477 | 0,003 | 0.0 |
| R | 5 | 28 | 4136,090 | 0,003 | 0.0 | R | 5 | 27 | 4135,683 | -0,001 | 0.0 |
| R | 5 | 26 | 4135,270 | 0,003 | 1.0 | R | 5 | 25 | 4134,834 | -0,001 | 1.0 |

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|---|---|---|---|---|---|---|---|---|---|---|
| R | 5 | 24 | 4134.395 | 0.009 | 0.0 | R | 5 | 23 | 4133.919 | -0.003 | 0.0 |
| R | 5 | 22 | 4133.446 | 0.002 | 0.1 | R | 5 | 21 | 4132.962 | 0.011 | 0.0 |
| R | 5 | 20 | 4132.445 | 0.004 | 0.3 | R | 5 | 19 | 4131.921 | 0.005 | 0.3 |
| R | 5 | 18 | 4131.378 | 0.001 | 0.0 | R | 5 | 17 | 4130.835 | 0.013 | 0.1 |
| R | 5 | 16 | 4130.245 | -0.006 | 0.0 | R | 5 | 15 | 4129.670 | 0.003 | 0.0 |
| R | 5 | 14 | 4129.072 | 0.006 | 0.0 | R | 5 | 13 | 4128.449 | -0.001 | 0.1 |
| R | 5 | 12 | 4127.813 | -0.006 | 0.0 | R | 5 | 11 | 4127.192 | 0.020 | 0.0 |
| R | 5 | 10 | 4126.528 | 0.017 | 0.0 | R | 5 | 9 | 4125.869 | 0.035 | 0.0 |
| R | 5 | 8 | 4125.188 | 0.046 | 0.0 | R | 5 | 7 | 4124.469 | 0.034 | 0.0 |
| R | 5 | 6 | 4123.732 | 0.019 | 0.0 | R | 5 | 5 | 4123.003 | 0.029 | 0.0 |
| R | 6 | 32 | 4136.622 | -0.006 | 0.1 | R | 6 | 31 | 4136.313 | 0.031 | 0.0 |
| R | 6 | 30 | 4135.923 | -0.001 | 0.3 | R | 6 | 29 | 4135.552 | 0.003 | 0.0 |
| R | 6 | 28 | 4135.154 | -0.005 | 0.0 | R | 6 | 27 | 4134.756 | 0.002 | 0.0 |
| R | 6 | 26 | 4134.324 | -0.010 | 0.0 | R | 6 | 25 | 4133.919 | 0.021 | 0.0 |
| R | 6 | 24 | 4133.446 | -0.002 | 0.0 | R | 6 | 23 | 4132.962 | -0.020 | 0.0 |
| R | 6 | 21 | 4132.005 | 0.001 | 0.7 | R | 6 | 20 | 4131.480 | -0.012 | 0.0 |
| R | 6 | 18 | 4130.408 | -0.016 | 0.0 | R | 6 | 17 | 4129.840 | -0.027 | 0.0 |
| R | 6 | 16 | 4129.280 | -0.015 | 0.3 | R | 6 | 15 | 4128.708 | 0.000 | 0.0 |
| R | 6 | 14 | 4128.103 | -0.003 | 0.0 | R | 6 | 13 | 4127.492 | 0.004 | 0.5 |
| R | 6 | 12 | 4126.857 | 0.002 | 0.5 | R | 6 | 11 | 4126.238 | 0.031 | 0.1 |
| R | 6 | 10 | 4125.583 | 0.040 | 0.1 | | | | | | |