

# Linelist of N<sub>2</sub>O parameters from 500 to 7500 cm<sup>-1</sup>

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## ABSTRACT

A new compilation of spectroscopic parameters of eight isotopic species of N<sub>2</sub>O has been generated from constants and coefficients given in previous studies. Also included are listings of the frequency constants and strength constants used to compute the line parameters included in the compilation. Air- and self-broadened half-width coefficients and pressure-induced frequency pressure-shift coefficients due to air-broadening are included in the compilation and these values were derived from measured data. The database contains 47,937 lines and covers the 525.462 to 7796.633 cm<sup>-1</sup> region with minimum line strengths of  $5.0 \times 10^{-6}$  cm<sup>-2</sup>/atm. at 296 K =  $2.02 \times 10^{-25}$  cm<sup>-1</sup>/(molecule-cm<sup>-2</sup>). The main listing is labeled SISAM.N2O and contains the computed parameters as well as experimental values for air-broadened widths and shifts with associated uncertainties and observed minus computed line positions for strongly perturbed (due to resonance interactions) transitions. The frequencies given in the listing for the perturbed transitions are the observed values. These listings are available from the author as well as a listing given in the HITRAN format.

## 1. INTRODUCTION

N<sub>2</sub>O is a trace constituent in the earth's atmosphere at a relative abundance of about  $2.7 \times 10^{-7}$  by volume near the earth's surface. An accurate knowledge of the spectroscopic parameters of N<sub>2</sub>O is important not only for deriving N<sub>2</sub>O concentrations in the troposphere and upper atmosphere but also for understanding the spectral features of other molecules located near N<sub>2</sub>O lines observed in atmospheric spectroscopic data. This study involves the listing of spectroscopic parameters of N<sub>2</sub>O that are applicable for atmospheric remote sensing. For this purpose, the database consists of computed values of transition frequencies, and strengths, and smoothed values of linewidths, and pressure-induced frequency shifts for the infrared region from 525 to 7796 cm<sup>-1</sup>.

Several studies have been reported on this subject and the relevant publications [1-58] are listed, in the references, in chronological order of publication date. The computed or smoothed values given in the present work are based on previous experimental studies [26,29,31,36,40,50,51] by this author. Briefly, the measurements were obtained at high spectral resolution with gas samples at room temperature. The line frequencies and strengths were derived from low pressure spectra with absorption path lengths up to 433 m [26,29,31,36,40,50]. The self-broadened data [40] covered the 1800 to 2360 cm<sup>-1</sup> region whereas the air-broadened measurements [51] (1800-4800 cm<sup>-1</sup>) included over 500 lines.

Recent work of note includes the following studies. Johns et al. [45] measured and analyzed line strengths of the  $\nu_2$  band in the 17  $\mu\text{m}$  region and the results differ somewhat from the HITRAN [57] values. Margottin-Maclou et al. [46] obtained air-broadened frequency shifts of N<sub>2</sub>O for transitions from measurements in the  $\nu_3$  band in the 2200 cm<sup>-1</sup> region. Daumont et al. [53] measured more than 3000 line strengths in 66 bands in the 3788-5319 cm<sup>-1</sup> region and

Nemtchinov et al. [56] measured strengths and air-broadened widths at temperatures of 216, 250, and 296K for observations in the  $\nu_3$  band.

The HITRAN compilation [57] contains 26,175  $\text{N}_2\text{O}$  transitions covering the 0.838 to 5131.249  $\text{cm}^{-1}$  region (451 lines below 523  $\text{cm}^{-1}$ ) with a minimum line strength cutoff of  $1.0 \times 10^{-25} \text{ cm}^{-1} / (\text{molecule}\cdot\text{cm}^{-2})$ . The HITRAN,  $\text{N}_2\text{O}$  listing includes five isotopic variants and does not contain self-broadened width coefficients and air-broadened frequency-shift coefficients. In contrast, the present  $\text{N}_2\text{O}$  listing, labeled, SISAM. $\text{N}_2\text{O}$ , contains 47,937 transitions and includes eight isotopic species with values given for all parameters for transitions up to 7796  $\text{cm}^{-1}$ . However the minimum line strength included in the present listing is 2 times larger than in the HITRAN counterpart. Considering the atmospheric  $\text{N}_2\text{O}$  concentration mentioned above and methods for calculating atmospheric  $\text{N}_2\text{O}$  optical densities, the weakest lines found in the present listing will not be observed in any IR atmospheric spectroscopic data. In addition, all  $\text{N}_2\text{O}$  features that can be observed in atmospheric spectra are represented in the present listing for transitions above 525  $\text{cm}^{-1}$  which is not the case for the HITRAN database since several of the vibrational bands included in the present listing are missing in the HITRAN list.

## 2. FREQUENCY PARAMETERS

The vibration-rotation energy can be expressed in terms of effective parameters:

$$E_v = G_v + B_v X - D_v X^2 + H_v X^3 + L_v X^4$$

$$X = J(J+1) \quad (1)$$

where  $G_v$  is the effective vibrational energy. Values of the parameters have been derived from analysis and are given for various vibrations in refs. [29,31,36,50]. They are given together here in Table 1. The parameters are given without uncertainties and these details can be found in the

studies from which they originated. The uncertainties of the computed frequencies obtained from these parameters are, on the average,  $\pm 6 \times 10^{-5} \text{ cm}^{-1}$  for unperturbed transitions. As noted in the table, vibrational states labeled with a “P” denote that one or more levels of the state are perturbed and transition frequencies computed from the given constants will be inaccurate for those levels.

### 3. STRENGTH PARAMETERS

The strength parameters obtained from earlier studies [26,40,50] covered the spectral region from 900 to 7800  $\text{cm}^{-1}$ . These values are listed in Table 2 in terms of the band center frequencies, vibrational band strength,  $S_v$ , and the F-factor coefficients,  $a_1$  and  $a_2$ . The values of the bands listed for band centers below 900  $\text{cm}^{-1}$  include the  $\nu_2$  parameters of  $^{14}\text{N}_2^{16}\text{O}$  given by Johns et al. [45] and estimates for the other bands since research from the earlier work did not cover these bands. It should be noted however that the computed line frequencies for these bands are accurate. The band centers were calculated from the values of  $G_v$  given in Table 1.

The line strengths,  $S$ , were computed from these parameters using the expression:

$$S = S_v(\nu/\nu_o)L[1 - \exp(-\nu/kT)] \times \exp[-E_R''/kT]F/Q_R, \quad (2)$$

where  $\nu_o$  is the band center frequency,  $L$  is the square of the matrix element of the direction cosines connecting the upper state to the lower state,  $E_R''$  is the lower state rotational energy,  $k$  is the Boltzmann constant,  $T$  is the temperature,  $F$  is the F factor,  $Q_R$  is the rotational partition function.  $S_v$  is expressed by,

$$S_v = 8\pi^3 |R|^2 \nu_o \exp(-E_v''/kT)/(3hcTQ_v), \quad (3)$$

where  $h$  is Plank's constant,  $c$  is the speed of light,  $Q_v$  is the vibrational-partition function,  $E_v''$  is the lower state vibrational energy, and  $R$  is the matrix element of the rotationless electric-dipole moment.

$L$  for R-,P-, and Q-branch transitions are given by the following expressions:

$$\begin{aligned}
 L &= (m^2 - \ell^2)|m|, & \Delta J = \pm 1, \Delta \ell = 0, 2; \\
 L &= \ell^2(2J+1)/[J(J+1)], & \Delta J = 0, \Delta \ell = 0, 2; \\
 L &= (m+z)(m+z+1)/|m| & \Delta J = \pm 1, \Delta \ell = \pm 1; \\
 L &= (2J+1)(J-z)(J+z+1)/[J(J+1)], & \Delta J = 0, \Delta \ell = \pm 1; \\
 z &= |\ell''|(|\ell'| - |\ell''|), & (4)
 \end{aligned}$$

where  $m = J'' + 1$  for the R-branch ( $\Delta J = 1$ ),  $m = -J'$  for the P-branch ( $\Delta J = -1$ ),  $m = 0$  for the Q-branch,  $\ell$  is the vibrational angular momentum quantum number, and prime and double prime denotes upper and lower states, respectively. The F-factor expressions are given as:

$$\begin{aligned}
 F &= [1 + a_1 m + a_2 J'(J' + 1)]^2 f, \\
 f &= 1 & \Delta \ell = 0, \pm 1, \\
 f &= [J'(J' + 1)]^2 & \Delta \ell = 2,
 \end{aligned} \tag{5}$$

where  $\Delta \ell = 2$  applies to the “forbidden” bands: 0220(e)-0000, 0420(e)-0000, 1220(e)-0000, 0221(e)-0000, 2220(e)-0000, and 1221(e)-0000 of  $^{14}\text{N}_2^{16}\text{O}$ . Line frequencies and strengths were measured for P- and R-branch transitions in these bands [26,40,50]. The upper states of these bands interact through a non resonance Fermi-type perturbation with  $\ell=0$  states having the same  $\nu_1\nu_2\nu_3$  vibrational quantum numbers and thus “borrow” intensity from the allowed band. Such is not the case for the 0620(e)-0000 band of  $^{14}\text{N}_2^{16}\text{O}$  whose transitions are observed due to resonance interactions with like transitions in the 1001-0000 band. Several other bands also have transitions that are perturbed due to resonance interactions. These were discussed in refs. [36,40,50].

#### 4. LINEWIDTHS AND SHIFTS

The derivation of atmospheric N<sub>2</sub>O from remote spectroscopic measurements does not require an accurate assessment of the N<sub>2</sub>O self-broadened width coefficients due to the low content of N<sub>2</sub>O in the atmosphere. However this is not the case for the air-broadened width coefficients. These parameters have been measured in a few studies [21,24,32,51,56] of which three [24,51,56] were found to have the most accurate values. The linewidth coefficients,  $b^o(\text{air})$ , given in those studies are compared in the upper portion of Fig. 1 which shows excellent agreement between the three studies. Lacome et al. [24] obtained their results from measurements in the 4 and 8  $\mu\text{m}$  spectral regions whereas Nemtchinov et al. [56] measured transitions in the  $\nu_3$  band. Toth [51] obtained N<sub>2</sub>- and air-broadened linewidths and pressure-induced frequency-shifts of N<sub>2</sub>O from spectra of room temperature gas samples. Over 500 lines were measured between 1800 and 4800  $\text{cm}^{-1}$  and  $1 \leq |m| \leq 73$  with accuracies of better than 2%, on the average. The measured  $b^o(\text{air})$  were fitted to a smoothing function expressed as:

$$b^o_{\text{smoothed}}(\text{air}) = B \exp[\sum_i b_i x_i], \quad (6)$$

where  $B=1\text{cm}^{-1}/\text{atm.}$  and  $x_i = |m|^{i-1}$ . The coefficients,  $b_i$ , that apply for  $|m| \leq 73$  have the following values:

$$b_1 = -2.324$$

$$b_2 = -2.214 \times 10^{-2}$$

$$b_3 = 5.671 \times 10^{-4}$$

$$b_4 = -6.716 \times 10^{-6}$$

$$\text{and} \quad b_5 = -2.614 \times 10^{-8}. \quad (7)$$

The smoothed values of  $b^o(\text{air})$  were also included in the plot given in the upper portion of Fig.1 and the curve fits well with the experimental data. The smoothed values of  $b^o(\text{air})$  at 296K were included in the compilations produced from this work.

The lower portion of Fig. 1 displays values of the exponent  $n$  for air-broadened widths derived from measurements [24,56] of  $b^o(\text{air})$  at various sample temperatures where  $n$  is given in the expression:

$$b^o(T) = b^o(T^o)[T^o/T]^n, \quad (8)$$

where  $b^o(T)$  is the width coefficient at sample temperature  $T$ . Also included in the figure are computed values [6] of  $n$  for  $\text{N}_2$  broadening of  $\text{N}_2\text{O}$  which should be close to air-broadened values. Inspection of the plots indicates that  $n$  may show a rotational trend however this is not conclusive from the measured values. By this token, an average value of  $n=0.75$  for all transitions was inserted in a new compilation given in HITRAN format. The uncertainty in  $n$  is about 10% as indicated from the figure which translates in an uncertainty in  $b^o(\text{air})$  at  $T=220\text{K}$  when derived from  $b^o(\text{air})$  at  $T=296\text{K}$  using eq. (6). This is certainly an acceptable condition for the analysis of atmospheric  $\text{N}_2\text{O}$  spectra. The broadening studies [24,51,56] also included measurements of  $\text{N}_2$  broadening of  $\text{N}_2\text{O}$  with similar accurate results.

The pressure-induced frequency-shift coefficients for air-broadening,  $d^o(\text{air})$ , were obtained for rotational transitions in 10 vibrational bands between  $1800$  and  $4800\text{ cm}^{-1}$  with values from about  $-0.001$  to almost  $-0.005\text{ cm}^{-1}/\text{atm}$ . [51]. The shift coefficients were found to have a weak  $J$  dependence in which the magnitude of  $d^o$  increased in proportion to  $J$  for a given vibrational band. The data were fitted to an empirical expression given as:

$$d^o(\text{air}) = d_1 + d_2 \times \left| m \right| + d_3 \times v,$$

$$\text{where } d_1 = 1.14 \times 10^{-3} \text{ cm}^{-1}/\text{atm}.$$



$$d_2 = -4.321 \times 10^{-5} \text{ cm}^{-1}/\text{atm.}$$

$$\text{and } d_3 = -9.517 \times 10^{-7} / \text{atm.} \quad (9)$$

where  $\nu$  is the transition frequency in  $\text{cm}^{-1}$ . Figure 2 shows the results for  $d^0(\text{air})$  for four bands with the computed values derived from eq. (9) as the dotted straight lines. Included in the figure are measurements obtained by Margottin-Maxlou et al. [46] which agree well with the computed values in the  $\nu_3$  band. The computed values of  $d^0(\text{air})$  were inserted in the compilations and these values are probably accurate to about 30% or better for the region below  $5000 \text{ cm}^{-1}$  and possibly as accurate above this region however no measurements have been reported.

## 5. LISTINGS

There are many transitions affected by interactions and are listed in Table 3. The list represents over 1200 transitions for the spectral region from  $577$  to  $7232 \text{ cm}^{-1}$  and limits the perturbed line strengths to  $5 \times 10^{-5} \text{ cm}^{-2}/\text{atm.}$  at  $296 \text{ K}$  ( $2.02 \times 10^{-25} \text{ cm}^{-1} / (\text{molecule-cm}^{-2})$ ). Obviously more transitions would be included in this list if the strength limit were lowered. Not only are the strengths altered for perturbed transitions but also the upper state energy levels and thus the line positions. The transition frequencies for perturbed lines were not treated with perturbation theory for this study however the line strengths of strongly perturbed lines were analyzed using perturbation theory as defined in ref. [40].

An example of the SISAM.N<sub>2</sub>O listing is given in Table 4. The compilation lists the molecule (M), isotopic species (I), line notation, lower state energy level, linewidth and shift coefficients, band notation, quantum line assignment, observed minus computed line position (o-c) and measured values of the air-broadening coefficients. The molecule and isotopic species notation is the same as that given for N<sub>2</sub>O in HITRAN [57]. The line notation was added to aid users and simply, it is the rotational line assignment without the letter R, P, or Q but may have a

different value than the value of the assignment value as defined at the bottom of the table. The line strengths are given in units of  $\text{cm}^{-2}/\text{atm.}$  at 296K whereas the HITRAN compilation lists strengths in  $\text{cm}^{-1}/(\text{molecule}\cdot\text{cm}^{-2})$  at 296K. The line positions are computed values derived from the constants given in Table 1 and using eq. (1) only for lines that are not perturbed. If a transition is perturbed, a value of o-c is given and the line position is the observed value. The self-broadened width coefficients were taken from ref. [40] and the air-broadened width and shift coefficients were computed from eqs. (6,7,9). The measured values of the air-broadening coefficients with uncertainties were taken from ref. [51]. The listing was also generated in HITRAN format but didn't include o-c and the measured broadening parameters.

## 6. CONCLUSION

A new compilation of infrared spectroscopic parameters for eight isotopic species of  $\text{N}_2\text{O}$  has been generated from constants, coefficients and measurements given in previous studies [26,29,31,36,40,45,50,51]. Also included are listings of the effective vibration-rotation constants, band centers, band strengths and F-factor coefficients used to compute the line parameters included in the compilation. Air- and self-broadened halfwidths and pressure-induced frequency pressure shifts due to air-broadening are included in the compilation and these values were derived from measured data. The database contains 47,937 lines and covers the 525.462 to 7796.633  $\text{cm}^{-1}$  region with minimum line strengths of  $5.0 \times 10^{-6} \text{ cm}^{-2}/\text{atm.}$  at 296 K =  $2.02 \times 10^{-25} \text{ cm}^{-1}/(\text{molecule}\cdot\text{cm}^{-2})$ . The main listing is labeled SISAM.N2O and contains the computed parameters as well as experimental values for air-broadened widths and shifts with associated uncertainties and observed minus computed line positions (o-c) for strongly perturbed (due to resonance interactions) transitions. The frequencies given in the listing for the perturbed

transitions are the observed values. Other listings also available are the following: a HITRAN formatted listing and Table 1 and Table 2. These listings are available on the website (<http://www.mark4sun.jpl.nasa.gov>).

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Table 1. Effective vibration-rotation constants ( $\text{cm}^{-1}$ ) of  $\text{N}_2\text{O}$  vibrational states used to compute transition frequencies in the SISAM.N2O listing

<i>mol</i>	<i>state</i>	$G_v$	$B_v$	$D_v$	$H_v$	$L_v$
558	0000e	0.	0.381865700	1.467300E-07		
548	0000e	0.	0.381919400	1.467000E-07		
547	0000e	0.	0.392781000	1.552000E-07		
458	0000e	0.	0.395467600	1.584000E-07		
448	0000e	0.	0.395577895	1.583456E-07		
546	0000e	0.	0.404857965	1.642938E-07	1.8666E-13	
556	0000e	0.	0.404860200	1.635600E-07		
457	0000e	0.	0.406608000	1.682000E-07		
447	0000e	0.	0.406672154	1.663972E-07		
456	0000e	0.	0.418981810	1.763264E-07		
446	0000e	0.	0.419011001	1.760919E-07	-1.6529E-14	
556	0110e	571.89400	0.405002100	1.656000E-07		
556	0110e	571.89400	0.405761700	1.663800E-07		
456	0110e	575.43365	0.419108916	1.785826E-07		
456	0110f	575.43365	0.419918641	1.794459E-07		
448	0110e	584.22466	0.395759697	1.600230E-07		
448	0110f	584.22466	0.396471172	1.610773E-07		
546	0110e	585.31212	0.405037265	1.656798E-07		
546	0110f	585.31212	0.405781109	1.667421E-07		
447	0110e	586.36197	0.406847000	1.683000E-07		
447	0110f	586.36197	0.407599000	1.713000E-07		
446	0110e	588.76787	0.419177925	1.783245E-07	-1.7140E-14	
446	0110f	588.76787	0.419969845	1.793030E-07	-1.7660E-14	
556	0200e	1136.45300	0.405741000	2.294000E-07		
456	0200e	1144.33338	0.419921722	2.845420E-07	6.6796E-12	
456	0220e	1151.03090	0.420032300	9.540000E-08		
456	0220f	1151.03090	0.420034800	1.813000E-07		
448	0200e	1155.13993	0.396278138	2.055029E-07	1.1670E-12	
546	0200e	1159.97171	0.405712750	2.227530E-07	2.2070E-12	
447	0200e	1161.54509	0.407485540	2.222920E-07	1.3828E-12	
446	0200e P	1168.13230	0.419920952	2.491945E-07	2.9554E-12	
448	0220e	1168.69790	0.396642600	1.315000E-07	-1.4000E-12	
448	0220f	1168.69790	0.396643700	1.640000E-07	1.0000E-13	
546	0220f	1170.84300	0.405950400	1.691000E-07		
546	0220e	1170.84300	0.405951200	1.218000E-07		
446	0220e	1177.74467	0.420125256	1.196792E-07	-2.9502E-12	-2.633E-17
446	0220f	1177.74467	0.420126260	1.818000E-07	9.5000E-14	-1.050E-17
448	1000e	1246.88456	0.394111338	1.495030E-07	3.4624E-13	
447	1000e	1264.70426	0.405053992	1.610001E-07	3.3710E-13	
556	1000e	1265.33383	0.403153720	1.627990E-07		
546	1000e	1269.89198	0.403263601	1.597707E-07	3.6343E-13	
456	1000e	1280.35412	0.417127307	1.754555E-07	4.7195E-14	
446	1000e	1284.90334	0.417255210	1.726978E-07	1.4666E-13	1.853E-18
448	0310f	1729.34712	0.397277403	1.933747E-07		
448	0310e	1729.34728	0.395988998	1.836498E-07		
546	0310e	1736.64780	0.405410775	1.914464E-07		
546	0310f	1736.64792	0.406798997	1.995707E-07		
446	0310f	1749.06515	0.421079073	2.177366E-07	-3.5921E-13	1.954E-17
446	0310e	1749.06523	0.419583944	2.110353E-07	1.2225E-12	-2.198E-17
446	0330f	1766.91224	0.420671366	1.683740E-07	3.0154E-12	
446	0330e	1766.91238	0.420667053	1.617863E-07	-9.9132E-13	
448	1110e	1839.93604	0.394349042	1.529218E-07	2.8186E-13	
448	1110f	1839.93604	0.395219127	1.472371E-07		
556	1110e	1842.40670	0.403318600	1.637500E-07		
556	1110f	1842.40670	0.404167000	1.620000E-07		
447	1110e	1858.76380	0.405283200	1.637440E-07		

Table 1. continued

<i>mol</i>	<i>state</i>	$G_v$	$B_v$	$D_v$	$H_v$	$L_v$
447	1110f	1858.76380	0.406171110	1.611420E-07		
456	1110e	1860.19121	0.417273136	1.773906E-07		
456	1110f	1860.19121	0.418165235	1.760323E-07		
546	1110e	1862.76708	0.403489655	1.609708E-07		
546	1110f	1862.76708	0.404358647	1.575290E-07		
446	1110e	1880.26574	0.417464677	1.748503E-07	1.0750E-13	
446	1110f	1880.26574	0.418372995	1.719561E-07	2.1746E-13	
558	0001e	2147.58500	0.378839400	1.462400E-07		
556	0001e	2154.72590	0.401617090	1.627970E-07	-8.7000E-14	
458	0001e	2171.04419	0.392360910	1.582150E-07	1.4100E-13	
457	0001e	2174.16420	0.403401000	1.685000E-07		
456	0001e	2177.65681	0.415654098	1.756773E-07	1.2541E-14	
548	0001e	2194.04555	0.378779050	1.462260E-07	-4.0000E-14	
547	0001e	2197.64860	0.389536000	1.543000E-07		
546	0001e	2201.60529	0.401497172	1.640337E-07	2.3380E-13	
448	0001e	2216.71118	0.392350601	1.579205E-07	1.2198E-14	
447	0001e	2220.07346	0.403340066	1.663531E-07	1.2850E-13	
446	0001e	2223.75677	0.415559510	1.754675E-07	-1.3626E-14	
456	0400e	2278.19266	0.420684310	5.029130E-07	3.0009E-11	
448	0400e	2294.01729	0.396795947	2.911980E-07	5.7265E-12	
546	0400e	2305.16257	0.406363987	3.382990E-07	9.8352E-12	
446	0400e P	2322.57308	0.420618918	3.964712E-07	1.4029E-11	2.064E-16
446	0420f	2331.12145	0.420772247	2.161040E-07	4.8397E-13	9.765E-18
446	0420e P	2331.12151	0.420768064	1.735120E-08	-1.4293E-11	-1.504E-16
446	0440e	2356.25242	0.421218620	2.720100E-07	1.7128E-10	-8.510E-14
446	0440f	2356.25242	0.421218620	2.720100E-07	1.7128E-10	-8.510E-14
556	1200e	2409.45600	0.404073700	2.414800E-07	3.4200E-12	
448	1200e	2411.50672	0.394608454	2.039123E-07	1.0377E-12	
456	1200e	2431.32249	0.418090902	2.744112E-07	4.2985E-12	1.218E-16
448	1220f	2431.49020	0.395379300	1.525000E-07		
448	1220e	2431.49020	0.395380900	1.336000E-07		
447	1200e	2435.72722	0.405784430	2.247120E-07	3.6683E-12	
456	1220f	2439.59880	0.418286100	1.874700E-07	3.1770E-12	
456	1220e	2439.59910	0.418282900	1.047500E-07	2.4250E-12	
546	1200e	2439.62463	0.404060515	2.177559E-07	1.8634E-12	
546	1220e	2454.60580	0.404529300	1.221000E-07	-2.1000E-12	
546	1220f	2454.60610	0.404528500	1.612800E-07		
446	1200e	2461.99644	0.418147866	2.430198E-07	2.5907E-12	-1.623E-17
446	1220f	2474.79865	0.418531597	1.755149E-07	2.4411E-13	-7.325E-18
446	1220e	2474.79870	0.418530437	1.206247E-07	-2.6981E-12	-5.648E-18
448	2000e	2491.18700	0.392925728	1.278238E-07	1.2060E-12	
556	2000e	2523.25340	0.401487600	1.587100E-07	3.2300E-13	
447	2000e	2524.67253	0.403616714	1.454285E-07	7.2668E-13	
546	2000e	2534.53206	0.401815575	1.479775E-07	8.0003E-13	
456	2000e	2552.40823	0.415298035	1.727937E-07	1.9889E-13	
446	2000e	2563.33944	0.415605503	1.637508E-07	5.6854E-13	9.733E-18
556	0111e	2713.14460	0.401800300	1.648600E-07		
556	0111f	2713.14460	0.402544910	1.658300E-07		
456	0111e	2739.59805	0.415824755	1.776541E-07		
456	0111f	2739.59805	0.416619104	1.787460E-07		
546	0111e	2772.70270	0.401718382	1.650934E-07		
546	0111f	2772.70270	0.402447853	1.663171E-07		
448	0111e	2787.01684	0.392572124	1.591979E-07		
448	0111f	2787.01684	0.393272984	1.606549E-07		
447	0111e	2792.36829	0.403557790	1.688630E-07	3.2887E-13	
447	0111f	2792.36829	0.404295890	1.708660E-07		
446	0111e	2798.29260	0.415770899	1.775781E-07	-1.1162E-14	

Table 1. continued

<i>mol</i>	<i>state</i>	$G_v$	$B_v$	$D_v$	$H_v$	$L_v$
446	0111f	2798.29260	0.416547926	1.787226E-07	-1.5579E-14	
446	0510f P	2897.81342	0.422038393	2.743442E-07	-2.1970E-12	8.576E-17
446	0510e P	2897.81350	0.419861584	2.613309E-07	4.8308E-12	-8.168E-17
446	0530e	2914.04341	0.421221015	1.440529E-07	-1.1131E-11	
446	0530f	2914.04344	0.421234739	1.802792E-07	1.6740E-11	
448	1310f	2990.17608	0.395759349	1.952290E-07	2.4512E-12	
448	1310e	2990.17682	0.394346540	1.799270E-07	-5.3170E-13	
456	1310f	3003.31779	0.419343220	2.131570E-07	-7.0120E-12	
456	1310e	3003.31793	0.417666110	2.074240E-07	-2.4480E-12	
546	1310e	3020.09714	0.403726660	1.962610E-07	2.7520E-12	
546	1310f	3020.09798	0.405229330	1.958737E-07	-2.3250E-13	
446	1310e	3046.21287	0.417758699	2.093227E-07	1.1871E-12	-3.007E-17
446	1310f	3046.21287	0.419376209	2.142852E-07	-2.0537E-13	3.518E-17
446	1330f	3068.72053	0.419111742	1.646400E-07	2.9895E-12	
446	1330e	3068.72060	0.419107121	1.574276E-07	-1.1803E-12	
448	2110f	3093.35486	0.394228830	1.244958E-07	-8.9000E-14	
448	2110e	3093.35503	0.393125755	1.392304E-07	-1.3000E-14	
546	2110e	3135.58222	0.402061184	1.533367E-07	2.6693E-13	
546	2110f	3135.58222	0.403110961	1.417340E-07	-9.7000E-14	
456	2110f	3136.97794	0.416466099	1.688420E-07	-6.0000E-15	
456	2110e	3136.97810	0.415466013	1.744618E-07	2.1900E-14	
446	2110e	3165.85362	0.415845548	1.676687E-07	2.0591E-13	1.796E-17
446	2110f	3165.85362	0.416919208	1.584805E-07	5.9778E-13	5.366E-18
456	0201e	3295.46206	0.416670011	2.857513E-07	7.0977E-12	
456	0221f	3301.80058	0.416780800	1.805000E-07		
456	0221e	3301.80085	0.416779300	9.400000E-08		
546	0201e	3333.73929	0.402423892	2.225370E-07	2.2463E-12	
546	0221f	3344.11945	0.402661400	1.680400E-07		
546	0221e	3344.11945	0.402662200	1.213000E-07		
448	0201e	3344.40349	0.393109315	2.064257E-07	1.4240E-12	
447	0201e	3354.00671	0.404213155	1.961216E-07	-1.3667E-11	
448	0221e	3357.67600	0.393486600	1.317000E-07	-1.5300E-12	
448	0221f	3357.67600	0.393487700	1.635000E-07	1.4000E-13	
446	0201e	3363.97798	0.416546127	2.492196E-07	3.0920E-12	
446	0221f	3373.14126	0.416750079	1.809069E-07	5.6789E-14	-8.115E-18
446	0221e	3373.14140	0.416748424	1.176478E-07	-3.2622E-12	-1.211E-17
556	1001e	3394.16294	0.399900309	1.618443E-07	-2.0500E-14	
456	1001e P	3432.19307	0.413792030	1.744255E-07	-2.8600E-14	
448	1001e P	3434.97624	0.390862300	1.481533E-07	3.3500E-13	
546	0600e P	3443.64998	0.399879921	1.575051E-07	1.1670E-13	
546	1001e P	3443.64998	0.399879921	1.575051E-07	1.1670E-13	
447	1001e P	3456.63632	0.401697793	1.585780E-07	-1.8160E-13	
446	0600e P	3466.59975	0.421192628	6.298511E-07	4.4100E-11	3.190E-16
446	0620e P	3474.44972	0.421309410	-1.521453E-07	-3.9913E-11	-1.202E-15
446	0620f	3474.44996	0.421315010	2.619901E-07	1.1574E-12	6.915E-17
446	1001e P	3480.81920	0.413785728	1.722949E-07	2.1660E-13	
448	1400e	3555.67713	0.395078433	2.708841E-07	-1.3522E-12	
456	1400e	3568.51900	0.418804900	4.755000E-07	2.0100E-11	
546	1400e	3589.92834	0.404645809	3.190425E-07	6.3814E-12	
446	1400e	3620.94311	0.418779733	3.733442E-07	6.0325E-12	2.120E-15
446	1420e	3631.58972	0.419031158	3.417760E-08	-1.0873E-11	-2.628E-16
446	1420f	3631.58972	0.419032886	2.118767E-07	3.7046E-13	6.674E-17
448	2200e	3661.02369	0.392827309	2.015311E-07	1.8888E-12	
456	2200e	3709.81275	0.416264779	2.767430E-07	7.0415E-12	
546	2200e	3712.12854	0.402333302	2.148563E-07	1.7688E-12	
448	3000e	3735.37364	0.392175361	8.853989E-08	1.7005E-12	
446	2200e	3748.25171	0.416330649	2.387304E-07	2.4558E-12	-4.017E-17



Table 1. continued

<i>mol</i>	<i>state</i>	$G_v$	$B_v$	$D_v$	$H_v$	$L_v$
446	2220f	3766.05247	0.417045031	1.636055E-07	-2.1862E-13	9.201E-17
446	2220e	3766.05253	0.417045204	1.213249E-07	-2.8302E-12	
447	3000e	3781.64788	0.402504682	1.125308E-07		
546	3000e	3795.45089	0.400640839	1.229237E-07	1.7832E-12	
456	3000e	3816.47539	0.413525995	1.680168E-07	1.2498E-12	
446	3000e	3836.37104	0.414158818	1.425685E-07	1.1525E-12	7.801E-17
456	0311f	3852.16535	0.417898113	2.339417E-07	4.1404E-12	
456	0311e	3852.16539	0.416356997	2.068917E-07	-5.1648E-12	
546	0311e	3896.77589	0.402174114	1.963593E-07	2.1022E-12	
546	0311f	3896.77671	0.403527991	1.918935E-07	-3.6350E-12	
448	0311e	3905.18230	0.392862292	1.846560E-07	7.9200E-14	
448	0311f	3905.18305	0.394123435	1.812007E-07	-7.4837E-12	
446	0311f	3931.24747	0.417728648	2.180777E-07	-1.6211E-13	
446	0311e	3931.24766	0.416262068	2.104143E-07	1.2210E-12	-1.277E-17
446	0331f	3948.28456	0.417336147	1.677448E-07	3.3789E-12	
446	0331e	3948.28475	0.417331757	1.614372E-07	-9.7299E-13	
456	1111e	3998.57148	0.413992363	1.785911E-07	6.2580E-13	
456	1111f	3998.57154	0.414860130	1.773694E-07	8.4730E-13	
448	1111e	4014.33138	0.391150488	1.493454E-07	-4.9720E-13	
448	1111f	4014.33171	0.392003962	1.453930E-07	2.0070E-13	
546	1111f	4022.28988	0.401006266	1.547679E-07	-6.3650E-13	
546	1111e	4022.29004	0.400160176	1.568285E-07	-9.2610E-13	
447	1111e	4038.00000	0.401998000	1.600000E-07		
447	1111f	4038.00000	0.402898000	1.600000E-07		
446	0730f P	4061.97956	0.414934474	1.707180E-07	1.3112E-13	
446	0710f P	4061.97956	0.414934474	1.707180E-07	1.3112E-13	
446	1111f P	4061.97956	0.414934474	1.707180E-07	1.3112E-13	
446	0730e P	4061.97960	0.414050142	1.739101E-07	2.0579E-13	
446	1111e P	4061.97960	0.414050142	1.739101E-07	2.0579E-13	
446	1510f	4197.96374	0.420255166	2.709689E-07	-1.0018E-12	
446	1510e	4197.96385	0.417939709	2.579649E-07	4.0207E-12	
446	1530f	4217.61977	0.419505990	1.519610E-07	-4.2614E-12	
446	1530e	4217.61977	0.419505990	1.519610E-07	-4.2614E-12	
456	2310e	4283.96194	0.415723720	6.089811E-08	-1.4363E-10	
456	2310f	4283.96667	0.417494404	1.446894E-08	-1.5843E-10	
546	2310e	4296.71503	0.402075236	3.033071E-07	7.9200E-11	
546	2310f	4296.71974	0.403676253	2.089839E-07	1.0857E-11	
456	0002e	4326.61717	0.412317083	1.748183E-07		
446	2310f	4335.79960	0.417682041	2.105275E-07	3.2791E-13	
446	2310e	4335.79969	0.415924084	2.060836E-07	9.1204E-13	
446	2330e	4364.62559	0.417642711	1.513535E-07	-1.2036E-12	
446	2330f	4364.62559	0.417642711	1.513535E-07	-1.2036E-12	
546	0002e	4373.60609	0.398130258	1.630547E-07		
448	0002e	4403.02759	0.389117140	1.580975E-07		
546	3110e	4404.83789	0.400795308	1.330704E-07	-8.6329E-12	
546	3110f	4404.84004	0.402089120	8.770653E-08	-1.7449E-11	
456	3110f	4406.12709	0.414864194	1.735184E-07	9.7101E-12	
456	3110e	4406.13044	0.413715895	2.003166E-07	1.3777E-11	
447	0002e	4409.92857	0.399996168	1.625025E-07		
446	0002e	4417.37776	0.412100231	1.749735E-07		
446	3110f	4446.38249	0.415670810	1.366574E-07	1.1387E-12	1.682E-17
446	3110e	4446.38251	0.414362431	1.559105E-07	4.6854E-13	4.688E-17
446	0401e	4491.54211	0.417319682	3.944600E-07	1.2536E-11	7.148E-16
446	0421f	4499.69374	0.417475225	2.156380E-07	6.4716E-13	-4.702E-17
446	0421e	4499.69405	0.417471152	1.598660E-08	-1.4922E-11	-1.146E-16
446	0441e	4523.70508	0.417935560	3.272300E-07	2.7399E-10	-1.440E-13
446	0441f	4523.70508	0.417935560	3.272300E-07	2.7399E-10	-1.440E-13

Table 1. continued

<i>mol</i>	<i>state</i>	$G_v$	$B_v$	$D_v$	$H_v$	$L_v$
456	1201e	4556.76685	0.414835533	2.632659E-07		
448	1201e	4572.49047	0.391392033	1.974968E-07	-2.6284E-12	
546	1201e	4585.67001	0.400763545	2.225172E-07	5.0972E-12	
446	0800e P	4616.12454	0.421692600	1.000600E-06	7.0000E-11	4.300E-16
446	1201e P	4630.16115	0.414761758	2.405560E-07	2.1234E-12	5.309E-17
446	1221e	4642.46220	0.415150953	1.208066E-07	-2.6145E-12	1.733E-17
446	1221f	4642.46222	0.415150379	1.739224E-07	2.2570E-13	
448	2001e	4650.54282	0.389683143	1.232991E-07	9.3298E-13	
456	2001e	4677.79785	0.411950301	1.689002E-07	-7.7134E-13	
546	2001e	4679.91818	0.398417775	1.462792E-07	9.6467E-13	
446	2001e	4730.82505	0.412118560	1.620142E-07	5.2662E-13	1.736E-17
446	1600e	4767.14211	0.419275157	5.937401E-07	3.1532E-11	1.458E-15
446	1620e	4777.00000	0.419400000	1.000000E-08		
446	1620f	4777.00000	0.419460000	2.000000E-07		
456	0112f	4875.06565	0.413312999	1.796632E-07		
456	0112e	4875.06578	0.412533725	1.787208E-07		
446	2400e	4910.99555	0.416899659	3.603352E-07	8.1753E-12	3.790E-16
446	2420e	4924.58806	0.417318880	5.140211E-08	-9.1774E-12	
446	2420f	4924.58878	0.417322105	2.100242E-07	1.7108E-12	
546	0112e	4930.51790	0.398395000	1.650700E-07		
546	0112f	4930.51790	0.399110900	1.658600E-07		
546	3200e	4976.64973	0.400489130	2.021174E-07		
446	0112f	4977.69769	0.413119986	1.784099E-07		
446	0112e	4977.69774	0.412356289	1.770458E-07		
456	3200e	4979.70261	0.414391046	2.474533E-07		
446	3200e	5026.30292	0.414404152	2.349362E-07	2.7516E-12	-6.199E-17
446	3220f	5052.10690	0.415705856	1.692656E-07	1.2799E-11	-2.440E-15
446	3220e	5052.10797	0.415694046	1.243737E-07	-3.9228E-12	
446	0511e	5053.58639	0.416632363	2.695296E-07	9.1185E-12	
446	0511f	5053.58719	0.418752363	2.681055E-07	-5.6026E-12	
546	4000e	5054.90941	0.399864710	7.695416E-08		
446	0531e	5069.07488	0.417973678	1.605020E-07	-4.2718E-12	4.268E-15
456	4000e	5073.06705	0.411861029	1.491165E-07		
446	4000e	5105.67692	0.413053603	1.049090E-07	2.8332E-12	1.232E-16
446	1311f P	5200.78110	0.416009836	2.126903E-07	-9.7124E-13	3.433E-16
446	1311e P	5200.78129	0.414433931	2.015722E-07	-3.8434E-12	1.022E-15
446	0910e P	5200.78129	0.414433931	2.015722E-07	-3.8434E-12	1.022E-15
446	1331e	5222.47037	0.415774377	1.550472E-07	-1.3265E-12	
456	2111e	5248.94870	0.412187700	1.758000E-07	1.2000E-12	
456	2111f	5248.94870	0.413154200	1.679000E-07		
546	2111e	5266.71610	0.398738000	1.507000E-07		
546	2111f	5266.71610	0.399751700	1.397500E-07		
446	2111f	5319.17369	0.413472279	1.568945E-07	7.2784E-13	
446	2111e	5319.17374	0.412431907	1.658197E-07	3.3123E-13	
446	2510f	5489.62162	0.418449192	2.712800E-07	1.8660E-12	
446	2510e	5489.62186	0.415979521	2.527556E-07	2.6847E-12	
446	0202e	5529.69497	0.413164931	2.490868E-07	3.1107E-12	
446	0222e	5538.43721	0.413365633	1.154332E-07	-3.7826E-12	
446	0222f	5538.43748	0.413367270	1.797653E-07	-2.2649E-13	
456	1002e	5555.64600	0.410449000	1.724000E-07		
446	0601e P	5609.82000	0.417700000	6.500000E-07		
446	0621e P	5617.76841	0.414080525	1.786311E-07	-1.5338E-11	4.939E-15
446	3310e P	5617.76841	0.414080525	1.786311E-07	-1.5338E-11	4.939E-15
446	0621f P	5617.76978	0.415984177	1.713653E-07	-1.3980E-11	2.545E-15
446	3310f P	5617.76978	0.415984177	1.713653E-07	-1.3980E-11	2.545E-15
446	1002e	5646.74019	0.410308009	1.711981E-07	1.9197E-13	
446	4110f	5722.82366	0.414679182	1.069720E-07	2.4392E-12	-1.673E-16

Table 1. continued

<i>mol</i>	<i>state</i>	$G_v$	$B_v$	$D_v$	$H_v$	$L_v$
446	4110e	5722.82375	0.413044803	1.378906E-07	-4.2676E-13	5.396E-16
446	1401e	5762.37267	0.415474313	3.708451E-07	1.0196E-11	
446	1421f	5772.62317	0.415735318	2.130187E-07	2.2824E-12	
446	1421e	5772.62356	0.415730293	3.234553E-08	-1.3393E-11	
446	2201e	5888.10587	0.412930176	2.372173E-07	2.2174E-12	
446	2221e	5905.41116	0.413681527	1.267444E-07	-1.2949E-12	3.964E-16
446	2221f	5905.41125	0.413682268	1.691909E-07	2.2536E-12	
546	3001e	5911.94814	0.397242056	1.060719E-07		
456	3001e	5914.70926	0.410158758	1.453565E-07		
446	3001e	5974.84507	0.410671277	1.364569E-07	-2.5919E-13	
446	2600e	6058.66749	0.417311176	5.651465E-07	2.9821E-11	
446	0312e	6107.80000	0.412500000	2.100000E-07	2.8000E-12	
446	0312f	6107.80000	0.414000000	2.100000E-07	1.0000E-12	
446	0332e	6125.00000	0.414100000	1.660000E-07		
446	3400e	6192.27059	0.414930148	3.467397E-07	8.9075E-12	
446	3420e	6210.21148	0.415645463	1.056115E-07	4.4339E-11	
446	1112f P	6213.81669	0.411490477	1.711460E-07	4.1896E-13	
446	0711f P	6213.81669	0.411490477	1.711460E-07	4.1896E-13	
446	0711e P	6213.81722	0.410624485	1.712273E-07	1.5145E-13	
446	1112e P	6213.81722	0.410624485	1.712273E-07	1.5145E-13	
446	4200e	6295.44763	0.412409340	2.159055E-07	4.0865E-12	
446	4220f	6333.51726	0.414486096	1.156051E-07	-8.4062E-12	
446	4220e	6333.51742	0.414483895	1.148334E-07	-2.2745E-11	
446	5000e	6373.30771	0.412345251	5.261853E-08	5.1625E-12	
446	2311f	6462.06892	0.414318604	2.263860E-07	5.7228E-12	
446	2311e	6462.06958	0.412610652	2.040505E-07	-1.7313E-12	
446	3111e	6570.76817	0.410970427	1.511749E-07	4.0842E-13	
446	3111f	6570.76824	0.412236464	1.307543E-07	6.9235E-13	
446	0003e	6580.85370	0.408635527	1.745407E-07		
446	1202e	6768.50167	0.411365722	2.391409E-07	5.0524E-12	
446	2002e	6868.54982	0.408629187	1.697666E-07	5.8930E-12	
446	0113f	7126.97880	0.409689927	1.786734E-07		
446	0113e	7126.97881	0.408936885	1.764348E-07		
446	3201e	7137.12706	0.410968484	2.307091E-07		
446	4001e P	7214.67990	0.409615412	9.034187E-08		
446	1003e	7782.66155	0.406826328	1.732056E-07	1.2761E-12	

The symbol P located after the state notation represents that one or more levels in the state are perturbed and frequencies computed from the constants will be inaccurate for the perturbed levels.

Vibrational state notation is as follows:  $v_1v_2\{v_3s$  where s is e or f

Table 2. Band centers ( $\text{cm}^{-1}$ ), sub-band strengths,  $S_V$  ( $\text{cm}^{-2}/\text{atm.}$  at 296K), F-factor coefficients,  $a_1$ ,  $a_2$ , and  $a_3$ , of  $\text{N}_2\text{O}$  used to compute rotational transition strengths that are given in the SISAM.N2O listing. Also included are number of transitions,  $N$ , minimum and maximum transition frequencies, number of sub-bands,  $N_s$ , and number of transitions measured to obtain air-broadening coefficients, NB.

<i>mol</i>	<i>band</i>	<i>band center</i>	<i>S<sub>V</sub></i>	<i>a<sub>1</sub>(e←e)</i>	<i>a<sub>1</sub>(f←f)</i>	<i>a<sub>2</sub>(e←e)</i>	<i>a<sub>2</sub>(f←f)</i>	<i>a<sub>3</sub>(f←e)</i>	<i>a<sub>3</sub>(e←f)</i>	<i>N</i>	<i>line</i>	<i>min.frq</i>	<i>line</i>	<i>max.frq.</i>	<i>N<sub>s</sub></i>	<i>NB</i>
446	0420	0330	564.2092	1.800E-03	2.50E-03	2.50E-03	0.00E+00	0.00E+00	0.00E+00	228	P38	532.3142	R40	599.1915	4	
456	0200	0110	568.8997	2.200E-03	2.50E-03		0.00E+00		0.00E+00	126	P39	537.2452	R43	606.9663	2	
448	0200	0110	570.9153	1.200E-03	2.50E-03		0.00E+00		0.00E+00	113	P35	543.7940	R39	603.2681	2	
446	0310	0220	571.3205	1.590E-02	2.50E-03	2.50E-03	0.00E+00	0.00E+00	0.00E+00	316	P51	526.6326	R54	619.9967	4	
446	0400	0310	573.5079	2.000E-03	2.50E-03		0.00E+00		0.00E+00	124	P38	542.7903	R42	610.9100	2	
546	0200	0110	574.6596	2.200E-03	2.50E-03		0.00E+00		0.00E+00	128	P40	543.2223	R43	611.3773	2	
456	0110	0000	575.4336	4.410E-02	2.50E-03		0.00E+00		0.00E+00	174	P55	529.8206	R59	625.9941	2	
456	0220	0110	575.5973	2.550E-03	2.50E-03	2.50E-03	0.00E+00	0.00E+00	0.00E+00	250	P39	543.0542	R44	615.5198	4	
446	0200	0110	579.3644	6.080E-01	2.50E-03		0.00E+00		0.00E+00	205	P66	526.3561	R70	640.9757	2	
446	0310	0200	580.9329	7.430E-02	2.50E-03		0.00E+00		0.00E+00	181	P58	531.6426	R61	631.9393	2	
446	1200	1110	581.7307	1.000E-03	2.50E-03		0.00E+00		0.00E+00	107	P33	554.8515	R37	614.2905	2	
446	0420	0310	582.0563	3.000E-03	2.50E-03	2.50E-03	0.00E+00	0.00E+00	0.00E+00	256	P40	547.9544	R45	623.8831	4	
448	0110	0000	584.2247	2.440E-02	2.50E-03		0.00E+00		0.00E+00	171	P54	542.1086	R58	631.3953	2	
448	0220	0110	584.4732	1.400E-03	2.50E-03	2.50E-03	0.00E+00	0.00E+00	0.00E+00	231	P36	556.1703	R41	619.3489	4	
546	0110	0000	585.3121	4.410E-02	2.50E-03		0.00E+00		0.00E+00	177	P56	540.6165	R60	635.2048	2	
546	0220	0110	585.5309	2.500E-03	2.50E-03	2.50E-03	0.00E+00	0.00E+00	0.00E+00	256	P40	553.3694	R45	624.9108	4	
447	0110	0000	586.3620	4.840E-03	2.50E-03		0.00E+00		0.00E+00	142	P44	550.9555	R48	626.5545	2	
446	0110	0000	588.7679	1.220E+01	2.50E-03		0.00E+00		0.00E+00	238	P77	525.4623	R80	657.2830	2	
446	0220	0110	588.9768	6.980E-01	2.50E-03	2.50E-03	0.00E+00	0.00E+00	0.00E+00	409	P66	534.3775	R70	654.2101	4	
446	0330	0220	589.1676	5.940E-02	2.50E-03	2.50E-03	0.00E+00	0.00E+00	0.00E+00	344	P56	543.5368	R61	643.6006	4	
446	0440	0330	589.3401	2.500E-03	2.50E-03	2.50E-03	0.00E+00	0.00E+00	0.00E+00	234	P38	558.1044	R44	627.7750	4	
446	1220	1110	594.5329	1.800E-03	2.50E-03	2.50E-03	0.00E+00	0.00E+00	0.00E+00	236	P37	563.8130	R42	632.5709	4	
446	1110	1000	595.3624	2.680E-02	2.50E-03		0.00E+00		0.00E+00	168	P53	551.7958	R57	644.3196	2	
446	1000	0110	696.1355	3.670E-02	0.00E+00		0.00E+00		0.00E+00	172	P56	643.4492	R57	738.1140	2	
446	1110	0220	702.5211	1.800E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	238	P40	664.6705	R39	733.2364	4	
446	1110	0200	712.1334	2.400E-03	0.00E+00		0.00E+00		0.00E+00	128	P41	673.9257	R42	743.7696	2	
446	0111	1110	918.0269	2.390E-03	-6.92E-04	-1.72E-04	6.95E-05	5.03E-05	6.00E-05	173	P43	878.7818	R44	952.0162	4	
446	0001	1000	938.8534	2.000E-02	-2.85E-04		1.79E-04			118	P58	884.9437	R59	982.5240	1	
446	0111	0310	1049.2274	8.225E-04	-2.77E-04	3.26E-04	3.85E-05	4.23E-05		128	P34	1015.5940	R35	1074.3760	2	
446	0001	0200	1055.6245	6.590E-03	-8.50E-05		8.65E-05			101	P50	1003.4648	R50	1087.2269	1	
456	0200	0000	1144.3334	1.090E-02	-2.07E-04		2.58E-05			104	P51	1103.4947	R52	1190.6007	1	
448	0310	0110	1145.1225	2.545E-03	-1.30E-04	-2.40E-04	0.00E+00	0.00E+00		171	P43	1111.4752	R43	1181.4268	2	
446	0530	0330	1147.1311	2.605E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00		160	P42	1112.7985	R43	1185.2712	2	
446	0510	0310	1148.7483	4.295E-03	-1.90E-04	4.30E-04	1.68E-05	4.40E-05	0.00E+00	187	P46	1110.6174	R47	1190.9964	4	
546	0310	0110	1151.3357	2.590E-03	-1.90E-04	-3.10E-04	0.00E+00	0.00E+00		170	P43	1117.1457	R43	1188.8744	2	
446	0420	0220	1153.3768	4.180E-02	-1.64E-04	-1.12E-03	2.16E-05	3.10E-05	0.00E+00	278	P58	1106.5610	R58	1205.8822	4	
446	0400	0200	1154.4408	5.910E-02	-7.30E-05		1.95E-05			120	P59	1106.2126	R60	1206.6201	1	
448	0200	0000	1155.1399	3.160E-02	1.50E-05		3.54E-05			118	P58	1111.2182	R59	1204.4609	1	
546	0200	0000	1159.9717	2.840E-02	1.14E-04		3.38E-05			116	P57	1116.1375	R58	1209.9938	1	
446	0310	0110	1160.2973	6.338E-01	-1.48E-04	-2.05E-04	1.43E-05	2.79E-05	0.00E+00	344	P69	1103.9876	R69	1223.3804	4	
447	0200	0000	1161.5451	4.030E-03	7.60E-05		0.00E+00			92	P45	1126.4074	R46	1201.2696	1	
446	1310	1110	1165.9471	1.728E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	158	P39	1133.7897	R40	1201.8066	4	
446	0200	0000	1168.1323	7.000E+00	-1.00E-06		2.48E-05			156	P78	1106.5732	R78	1237.5697	1	
446	1200	1000	1177.0931	2.260E-02	3.21E-04		3.84E-05			112	P55	1133.4030	R56	1226.8015	1	
446	0220	0000	1177.7447	5.530E-08	-1.57E-04		0.00E+00			127	P71	1125.0525	R72	1245.8266	1	
448	2000	1000	1244.3024	1.000E-03	0.00E+00		0.00E+00			70	P36	1214.4965	R37	1272.5156	1	
448	1000	0000	1246.8846	4.140E-01	0.00E+00		0.00E+00			138	P68	1186.8198	R69	1295.0204	1	
448	1110	0110	1255.7114	2.305E-02	-2.24E-04	-2.00E-04	-4.30E-06	-2.20E-06	0.00E+00	246	P56	1207.2295	R56	1296.8018	4	
448	1200	0200	1256.3668	1.510E-03	0.00E+00		0.00E+00			78	P39	1223.0338	R40	1285.9346	1	
446	1001	0001	1257.0624	4.440E-03	0.00E+00		0.00E+00			93	P46	1215.2504	R46	1292.0642	1	

Table 2. continued

<i>mol</i>	<i>band</i>	<i>band center</i>	<i>S<sub>V</sub></i>	<i>a<sub>1</sub>(e←e)</i>	<i>a<sub>1</sub>(f←f)</i>	<i>a<sub>2</sub>(e←e)</i>	<i>a<sub>2</sub>(f←f)</i>	<i>a<sub>3</sub>(f←e)</i>	<i>a<sub>3</sub>(e←f)</i>	<i>N</i>	<i>line</i>	<i>min. frq</i>	<i>line</i>	<i>max. frq.</i>	<i>N<sub>s</sub></i>	<i>NB</i>	
448	1220	0220	1262.7923	1.500E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00		148	P39	1230.0162	R40	1293.1282	2		
546	2000	1000	1264.6401	1.460E-03	0.00E+00		0.00E+00			77	P39	1231.1046	R39	1294.5194	1		
447	1000	0000	1264.7043	7.980E-02	0.00E+00		0.00E+00			123	P61	1209.4077	R61	1308.7549	1		
556	1000	0000	1265.3338	2.690E-03	0.00E+00		0.00E+00			87	P43	1227.4884	R43	1297.5299	1		
546	1000	0000	1269.8920	7.000E-01	-2.99E-04		0.00E+00			141	P70	1205.8601	R70	1319.1400	1		
456	2000	1000	1272.0541	1.600E-03	0.00E+00		0.00E+00			77	P39	1236.8551	R39	1302.3872	1		
447	1110	0110	1272.4018	4.535E-03	1.50E-04	-2.00E-05	1.23E-05	2.40E-05	0.00E+00	0.00E+00	191	P47	1231.1190	R47	1308.1534	4	
446	3000	2000	1273.0316	8.000E-04	0.00E+00		0.00E+00			62	P33	1244.1217	R34	1300.3082	1		
546	1110	0110	1277.4550	3.890E-02	7.90E-05	-1.50E-04	3.20E-06	6.60E-06	0.00E+00	0.00E+00	262	P58	1225.5350	R58	1320.2801	4	
446	2000	1000	1278.4361	7.910E-01	-2.14E-04		2.90E-06			140	P69	1213.5843	R70	1329.3031	1		
546	1200	0200	1279.6529	2.510E-03	0.00E+00		0.00E+00			84	P42	1242.8052	R43	1312.0274	1		
456	1000	0000	1280.3541	7.900E-01	0.00E+00		0.00E+00			139	P69	1214.0890	R69	1329.5801	1		
546	1220	0220	1283.7630	2.435E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00		164	P42	1247.2389	R43	1316.6444	2		
456	1110	0110	1284.7576	4.630E-02	-1.29E-04	-1.90E-05	8.30E-06	9.00E-06	0.00E+00	0.00E+00	266	P58	1230.2242	R58	1327.9963	4	
446	1000	0000	1284.9033	2.080E+02	-9.00E-06		0.00E+00			175	P87	1199.5871	R87	1344.7110	1		
446	2110	1110	1285.5879	4.300E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	262	P57	1233.0360	R58	1329.8557	4		
446	2200	1200	1286.2553	1.300E-03	0.00E+00		0.00E+00			74	P37	1252.9472	R38	1315.9894	1		
456	1200	0200	1286.9891	3.060E-03	0.00E+00		0.00E+00			88	P43	1247.6743	R44	1320.9205	1		
456	1220	0220	1288.5681	2.940E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00		166	P43	1249.3001	R43	1322.0169	2		
446	2220	1220	1291.2538	1.220E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00		138	P37	1258.3283	R37	1320.8458	2		
446	1110	0110	1291.4979	1.250E+01	-4.40E-05	-1.48E-04	-6.40E-06	-3.60E-06	0.00E+00	0.00E+00	412	P78	1216.3075	R79	1348.3504	4	
446	1200	0200	1293.8641	7.640E-01	-2.13E-04		-8.80E-06			139	P69	1227.9858	R69	1343.6266	1		
446	1220	0220	1297.0540	7.310E-01	-1.08E-04	-1.90E-05	-1.01E-05	-1.13E-05	-2.28E-05	-2.28E-05	352	P68	1232.8418	R69	1347.8725	4	
446	1310	0310	1297.1477	4.540E-02	-1.30E-05	-1.05E-04	-9.40E-06	-1.10E-05	0.00E+00	0.00E+00	260	P57	1243.6566	R57	1340.0434	4	
446	1400	0400	1298.3700	2.650E-03	-3.20E-04		-1.40E-05			85	P42	1260.0178	R42	1330.9973	1		
446	1420	0420	1300.4682	2.495E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00		162	P42	1262.1159	R42	1333.3111	2		
446	1330	0330	1301.8083	4.150E-02	2.00E-05	1.26E-04	-6.80E-06	-1.25E-05	-1.00E-05	-1.00E-05	277	P57	1249.0346	R57	1345.1923	4	
446	2000	0200	1395.2071	3.460E-03	1.53E-04		3.95E-05			91	P45	1349.2738	R45	1424.7920	1		
446	0201	0310	1614.9128	2.040E-04					0.00E+00	20	Q 7	1614.6589	Q26	1611.7164	1		
446	0111	0220	1620.5479	1.653E-03	6.20E-03	6.49E-03	-8.35E-05	1.16E-05	5.12E-05	-4.20E-06	234	P36	1585.8287	R43	1650.3834	4	
446	0111	0200	1630.1603	1.530E-03	6.64E-03		8.19E-05		-8.72E-05		120	P36	1594.8501	R44	1659.5556	2	
446	0001	0110	1634.9889	2.940E-02	6.21E-03		-3.50E-06		-6.27E-05		166	P51	1583.1191	R58	1671.5321	2	
446	0510	0200	1729.6812	2.940E-04	-5.70E-03		-3.00E-05		0.00E+00		47	P24	1709.5025	R15	1743.0976	2	
446	0400	0110	1733.8052	1.860E-03	-6.14E-03		1.29E-04		0.00E+00		130	P46	1697.4868	R40	1770.0367	2	
446	0530	0220	1736.2988	1.400E-04				0.00E+00	0.00E+00	14	Q13	1736.4988	Q19	1736.7196	2		
546	0310	0000	1736.6479	1.400E-04				0.00E+00		8	Q12	1736.9499	Q19	1737.3804	1		
446	0420	0110	1742.3536	1.660E-03	-4.52E-03	-5.26E-03	-1.26E-04	3.16E-05	0.00E+00	0.00E+00	232	P42	1708.4045	R38	1776.2328	4	
446	0310	0000	1749.0652	2.295E-02	-5.83E-03		2.31E-05		3.38E-05		168	P57	1702.9393	R52	1794.7566	2	
448	1110	0000	1839.9360	4.780E-04	-8.81E-03		2.64E-05		0.00E+00		81	P34	1811.6901	R23	1858.1797	2	
456	1110	0000	1860.1912	9.080E-04	-1.07E-02		3.65E-05		0.00E+00		106	P40	1824.0497	R29	1883.7211	2	
546	1110	0000	1862.7671	9.240E-04	-1.10E-02		-3.21E-05		-1.32E-05		104	P40	1828.2932	R27	1884.3157	2	
446	1310	0220	1868.4682	1.700E-04	-1.08E-02	-1.08E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	42	P19	1851.6871	Q41	1868.4682	4	
446	1200	0110	1873.2286	8.600E-03	-1.41E-02		8.14E-05		-1.13E-04		148	P56	1822.6944	R42	1907.0581	2	
446	1310	0200	1878.0806	1.160E-03	-1.44E-02		5.00E-06		-3.10E-05		109	P43	1838.2583	R27	1899.8441	2	
446	1110	0000	1880.2657	2.575E-01	-1.09E-02		-6.00E-07		-1.40E-06		194	P69	1815.4586	R57	1923.4615	2	19
446	2110	1000	1880.9503	1.030E-03	-1.11E-02		2.14E-05		0.00E+00		108	P41	1844.4849	R29	1904.6604	2	
446	1220	0110	1886.0308	1.460E-02	-1.07E-02	-1.16E-02	-5.64E-05	-9.00E-06	-2.18E-05	2.12E-05	303	P56	1834.7333	R43	1921.7810	4	
446	1330	0220	1890.9759	1.260E-03	-1.22E-02	-1.19E-02	-4.23E-05	-6.93E-05	0.00E+00	0.00E+00	208	P41	1854.7975	R29	1915.2375	4	
446	2000	0110	1974.5716	5.120E-03	-9.64E-03		1.80E-05		2.43E-05		143	P51	1922.9053	R41	2003.3289	2	
446	0201	1000	2079.0746	4.900E-04	-8.65E-04		0.00E+00			48	P29	2054.2660	R28	2102.5857	1		
556	0111	0110	2141.2506	9.190E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00		130	P35	2109.0486	R35	2166.1506	2		
456	0221	0220	2150.7698	1.560E-02	2.55E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	242	P52	2098.5231	R53	2186.4243	4	
456	0201	0200	2151.1287	1.570E-02	-2.50E-04		0.00E+00			106	P52	2098.9774	R53	2186.6621	1		

Table 2. continued

<i>mol</i>	<i>band</i>	<i>band center</i>	<i>S<sub>V</sub></i>	<i>a<sub>1</sub>(e←e)</i>	<i>a<sub>1</sub>(f←f)</i>	<i>a<sub>2</sub>(e←e)</i>	<i>a<sub>2</sub>(f←f)</i>	<i>a<sub>3</sub>(f←e)</i>	<i>a<sub>3</sub>(e←f)</i>	<i>N</i>	<i>line</i>	<i>min. frq</i>	<i>line</i>	<i>max. frq.</i>	<i>N<sub>s</sub></i>	<i>NB</i>	
456	1001	1000	2151.8390	7.310E-03	0.00E+00		0.00E+00			98	P48	2104.3523	R49	2184.9656	1		
556	0001	0000	2154.7259	1.550E-02	-2.61E-04		-1.69E-05			107	P53	2102.9741	R53	2188.7202	1		
456	0111	0110	2164.1644	2.620E-01	2.36E-04	1.87E-04	-3.90E-06	0.00E+00	0.00E+00	0.00E+00	318	P65	2096.0581	R65	2204.8104	4	
446	0441	0440	2167.4527	2.610E-02	0.00E+00		0.00E+00		0.00E+00	133	P55	2109.6889	R53	2200.2028	2		
446	2001	2000	2167.4856	3.700E-03	1.30E-04		4.40E-05			93	P46	2122.1022	R46	2198.6274	1		
446	1221	1220	2167.6635	7.380E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	214	P48	2119.9186	R49	2200.8346	4		
446	1201	1200	2168.1647	6.700E-03	-7.40E-04		-3.80E-05			95	P47	2121.6450	R47	2200.2515	1		
446	0421	0420	2168.5724	1.425E-02	4.80E-04	8.50E-04	-1.30E-05	-6.00E-06	0.00E+00	0.00E+00	236	P51	2117.2869	R52	2203.6894	4	
446	0401	0400	2168.9690	1.450E-02	-6.70E-04		-2.30E-05			104	P52	2116.6758	R51	2203.4448	1		
458	0001	0000	2171.0442	8.440E-03	0.00E+00		0.00E+00			102	P50	2123.9684	R51	2203.5261	1		
546	0221	0220	2173.2765	1.560E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	244	P53	2121.2575	R53	2207.2785	4		
546	1001	1000	2173.7580	8.430E-03	9.60E-04		0.00E+00			101	P49	2126.3636	R51	2206.2950	1		
546	0201	0200	2173.7676	1.570E-02	0.00E+00		0.00E+00			107	P53	2121.8275	R53	2207.6854	1		
456	0001	0000	2177.6568	4.210E+00	7.65E-05		2.20E-06			151	P75	2096.6604	R75	2221.5834	1	15	
446	0331	0330	2181.3723	2.240E-01	-1.06E-04	-1.06E-04	0.00E+00	0.00E+00	0.00E+00	324	P64	2114.2620	R64	2221.6278	4		
446	1111	1110	2181.7138	1.353E-01	0.00E+00	6.95E-04	0.00E+00	0.00E+00	0.00E+00	298	P62	2116.9997	R63	2220.7942	4		
446	0311	0310	2182.1824	2.500E-01	1.96E-04	6.50E-05	0.00E+00	0.00E+00	0.00E+00	316	P65	2114.0551	R65	2222.6998	4		
546	0111	0110	2187.3906	2.640E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	322	P66	2119.7274	R66	2226.3872	4		
448	1001	1000	2188.0917	5.710E-03	0.00E+00		0.00E+00			98	P48	2143.0014	R49	2219.1502	1		
448	0221	0220	2188.9781	8.900E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	226	P51	2140.5420	R51	2221.4496	4		
448	0201	0200	2189.2636	8.920E-03	0.00E+00		0.00E+00			103	P51	2140.8676	R51	2221.6287	1		
446	0620	1000	2189.5464	2.220E-10	3.92E-04		7.60E-06			2	P29	2168.8448	R27	2216.3800	1		
447	1001	1000	2191.9321	1.080E-03	0.00E+00		0.00E+00			70	P36	2158.5721	R37	2217.7107	1		
446	0002	0001	2193.6210	4.960E-02	-1.45E-04		-1.01E-05			117	P58	2134.1226	R58	2230.2738	1		
548	0001	0000	2194.0456	9.870E-03	0.00E+00		0.00E+00			105	P52	2146.0828	R52	2225.4569	1		
446	0221	0220	2195.3967	4.043E+00	-1.06E-04	-3.57E-05	-3.40E-06	-1.60E-06	0.00E+00	0.00E+00	394	P75	2113.9060	R75	2239.2602	4	1
446	0201	0200	2195.8457	4.240E+00	-5.84E-05		-1.96E-06			151	P75	2114.5283	R75	2239.5581	1	5	
446	1001	1000	2195.9159	2.220E+00	3.92E-04		7.60E-06			148	P73	2117.0476	R74	2238.4630	1	2	
546	0001	0000	2201.6053	4.420E+00	-5.89E-05		0.00E+00			154	P76	2121.2132	R77	2243.7662	1		
448	0111	0110	2202.7922	1.500E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	308	P64	2139.3245	R65	2240.8070	4		
447	0111	0110	2206.0063	2.860E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	250	P56	2150.3061	R56	2241.4304	4		
446	0111	0110	2209.5247	6.890E+01	-5.92E-05	-3.76E-05	2.28E-06	3.92E-06	0.00E+00	0.00E+00	448	P84	2115.5666	R84	2255.4963	4	5
448	0001	0000	2216.7112	2.450E+00	-9.70E-06		5.00E-06			152	P75	2139.7454	R76	2257.9759	1		
447	0001	0000	2220.0735	5.060E-01	-1.52E-04		0.00E+00			138	P68	2149.8074	R69	2260.2357	1		
446	0001	0000	2223.7568	1.240E+03	-2.25E-05		0.00E+00			185	P92	2118.3575	R92	2271.0023	1	9	
456	0400	0000	2278.1927	5.830E-04	0.00E+00		0.00E+00			54	P30	2254.3265	R31	2306.4534	1		
448	0400	0000	2294.0173	6.190E-03	-3.94E-04		0.00E+00			99	P49	2257.5296	R49	2335.8330	1		
446	0620	0220	2296.7052	5.410E-03	1.79E-04	-2.53E-04	2.61E-05	1.10E-05	1.50E-05	205	P47	2259.4966	R48	2341.7627	4		
446	0600	0200	2298.4675	8.720E-03	-2.57E-04		1.25E-05			101	P50	2258.0392	R50	2342.6418	1		
546	0400	0000	2305.1626	2.690E-03	-1.07E-04		1.97E-05			89	P44	2271.8827	R44	2343.9976	1		
446	0510	0110	2309.0456	6.993E-02	-2.67E-04	-1.64E-04	6.10E-06	1.80E-06	0.00E+00	0.00E+00	280	P60	2260.4746	R60	2366.4882	4	
446	0400	0000	2322.5731	5.800E-01	-1.86E-04		0.00E+00			137	P68	2269.9169	R68	2384.4850	1		
446	0420	0000	2331.1215	1.530E-08	1.75E-04		-7.23E-05			101	P61	2288.0017	R62	2392.4523	1		
446	1400	1000	2336.0398	1.670E-03	7.70E-04		2.68E-05			79	P39	2305.3810	R41	2373.1894	1		
448	1310	0110	2405.9518	2.395E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00		170	P43	2369.3475	R43	2439.2617	2		
448	1200	0000	2411.5067	3.680E-02	1.43E-04		3.07E-05			119	P59	2361.1492	R59	2454.7316	1		
456	1310	0110	2427.8842	9.490E-04	0.00E+00	1.17E-03	0.00E+00	0.00E+00		133	P35	2396.8154	R36	2458.0266	2		
456	1200	0000	2431.3225	1.000E-02	-5.90E-05		2.44E-05			103	P51	2385.8467	R51	2471.6941	1		
546	1310	0110	2434.7854	1.910E-03	1.73E-04	-4.29E-04	2.48E-05	4.96E-05		165	P41	2399.3981	R42	2468.4802	2		
447	1200	0000	2435.7272	3.950E-03	-4.07E-04		4.24E-05			95	P47	2395.4144	R47	2472.3313	1		
546	1200	0000	2439.6246	2.710E-02	-2.09E-04		3.86E-05			115	P57	2390.5562	R57	2483.1729	1		
446	1510	0310	2448.8986	3.435E-03	4.41E-04	-7.19E-04	2.60E-05	-4.70E-05	0.00E+00	0.00E+00	177	P44	2408.7863	R43	2484.0337	4	
446	1530	0330	2450.7075	1.990E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	168	P40	2415.2894	R41	2483.9106	4		

Table 2. continued

<i>mol</i>	<i>band</i>	<i>band center</i>	<i>S<sub>V</sub></i>	<i>a<sub>1</sub>(e←e)</i>	<i>a<sub>1</sub>(f←f)</i>	<i>a<sub>2</sub>(e←e)</i>	<i>a<sub>2</sub>(f←f)</i>	<i>a<sub>3</sub>(f←e)</i>	<i>a<sub>3</sub>(e←f)</i>	<i>N</i>	<i>line</i>	<i>min. frq</i>	<i>line</i>	<i>max. frq.</i>	<i>N<sub>s</sub></i>	<i>NB</i>	
446	1400	0200	2452.8108	4.970E-02	2.10E-04		1.06E-05			118	P58	2399.4184	R59	2497.5264	1		
446	1420	0220	2453.8451	3.468E-02	-6.70E-05	1.44E-04	1.77E-05	0.00E+00	0.00E+00	271	P57	2403.1471	R57	2499.3814	4		
446	2310	1110	2455.5339	2.505E-03	0.00E+00	-1.01E-03	0.00E+00	0.00E+00	0.00E+00	169	P42	2417.7772	R42	2490.0148	4		
446	1310	0110	2457.4450	5.233E-01	-1.31E-04	2.90E-05	1.40E-05	2.34E-05	2.00E-05	339	P68	2393.6527	R69	2512.1786	4	19	
446	1200	0000	2461.9964	6.690E+00	-7.60E-05		2.10E-05			156	P77	2390.9510	R78	2520.3566	1	84	
446	2200	1000	2463.3484	4.020E-02	4.40E-05		3.65E-05			117	P58	2411.3810	R58	2508.4387	1		
446	1220	0000	2474.7987	3.570E-08	5.89E-04		0.00E+00			121	P69	2415.8933	R70	2532.6768	1		
448	2000	0000	2491.1870	6.670E-02	0.00E+00		0.00E+00			123	P61	2433.8313	R61	2530.2659	1		
446	2001	0001	2507.0683	6.860E-04	0.00E+00		0.00E+00			59	P32	2477.0958	R32	2530.6270	1		
448	2110	0110	2509.1303	2.990E-03	-2.61E-04	-2.63E-04	5.28E-05	2.49E-05	0.00E+00	0.00E+00	182	P46	2467.4195	R45	2540.8650	4	
556	2000	0000	2523.2534	4.000E-04	0.00E+00		0.00E+00			41	P26	2500.0221	R27	2543.1760	1		
447	2000	0000	2524.6725	1.200E-02	0.00E+00		0.00E+00			105	P52	2474.5302	R52	2559.1248	1		
546	2000	0000	2534.5321	9.570E-02	0.00E+00		0.00E+00			125	P62	2473.2455	R62	2573.4195	1		
446	4000	2000	2542.3375	4.000E-04	0.00E+00		0.00E+00			41	P26	2519.1042	R26	2562.8727	1		
546	2110	0110	2550.2701	4.230E-03	-4.41E-04	5.39E-04	6.71E-05	2.84E-05	0.00E+00	0.00E+00	191	P48	2504.8117	R47	2583.0082	4	
446	3000	1000	2551.4677	1.580E-01	-7.70E-05		-7.90E-06			127	P63	2487.5082	R63	2592.4319	1	1	
456	2000	0000	2552.4082	9.920E-02	0.00E+00		0.00E+00			123	P61	2488.0270	R61	2589.8708	1		
456	2110	0110	2561.5444	5.008E-03	-7.34E-04	-2.28E-04	4.91E-05	3.60E-05	0.00E+00	0.00E+00	193	P48	2513.1918	R47	2593.7153	4	
446	2000	0000	2563.3394	3.000E+01	0.00E+00		0.00E+00			164	P81	2474.4613	R82	2609.5702	1	41	
446	3200	1200	2564.3065	4.000E-04	0.00E+00		0.00E+00			41	P26	2540.1497	R26	2584.0420	1		
446	3110	1110	2566.1168	7.020E-03	-6.36E-04	2.99E-04	3.33E-05	3.62E-05	0.00E+00	0.00E+00	204	P50	2516.9777	R50	2601.8001	4	
446	2110	0110	2577.0858	1.505E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	364	P71	2501.5576	R72	2622.3518	4	34	
446	3220	1220	2577.3088	4.000E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00		78	P26	2553.7088	R26	2597.7671	2		
446	2200	0200	2580.1194	8.200E-02	0.00E+00		0.00E+00			121	P60	2517.3234	R60	2617.6744	1		
446	2310	0310	2586.7345	4.200E-03	2.26E-04	-4.40E-05	1.77E-05	2.38E-05	0.00E+00	0.00E+00	185	P46	2541.0851	R46	2618.6054	4	
446	2220	0220	2588.3078	7.927E-02	-5.90E-05	7.80E-05	-7.00E-06	-2.00E-06	1.88E-05	0.00E+00	294	P60	2527.0960	R60	2628.0094	4	
446	2400	0400	2588.4225	4.000E-04	0.00E+00		0.00E+00			40	P25	2565.1957	R26	2608.3123	1		
446	2420	0420	2593.4669	4.000E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00		76	P25	2570.3494	R26	2613.5677	2		
446	2330	0330	2597.7133	8.390E-03	1.12E-04		-2.76E-05		0.00E+00	111	P48	2550.6300	R49	2632.0494	2		
446	3000	0200	2668.2387	1.720E-03	1.37E-04		4.92E-05			80	P40	2625.9712	R41	2693.3721	1		
456	0111	0000	2739.5981	3.245E-03	3.57E-04		2.19E-05	0.00E+00		137	P44	2696.8098	R45	2771.2440	2		
446	0401	0310	2742.4769	3.060E-04	0.00E+00		0.00E+00		1.17E-04	56	P22	2722.9400	R21	2759.7385	2		
446	0421	0310	2750.6287	2.615E-04	0.00E+00	0.00E+00	0.00E+00	-1.27E-04	4.61E-05	82	Q 5	2750.5208	R22	2768.8099	4		
446	0311	0220	2753.5029	1.385E-03	3.31E-03	3.54E-03	-2.00E-06	1.57E-04	4.18E-05	234	P40	2716.1097	R43	2785.5207	4		
446	0441	0330	2756.7928	7.150E-04	0.00E+00		0.00E+00		0.00E+00	87	P30	2729.1672	R34	2782.6941	2		
446	0311	0200	2763.1153	6.260E-03	3.86E-04		1.30E-05	-2.83E-05		146	P47	2715.9952	R48	2795.3979	2		
446	0331	0220	2770.5400	4.670E-03	3.47E-04	4.67E-04	-1.56E-05	-1.62E-05	-1.07E-05	266	P44	2728.1918	R46	2803.7714	4		
546	0111	0000	2772.7027	3.290E-03	3.18E-04		2.16E-05	0.00E+00		140	P45	2730.1042	R46	2803.6023	2		
446	0201	0110	2775.2101	5.390E-02	7.97E-04		5.59E-05		-7.95E-05	179	P60	2714.9958	R61	2815.8419	2		
446	1111	1000	2777.0762	1.850E-03	-3.22E-04		4.76E-05	-2.44E-05		125	P41	2737.6495	R41	2806.2827	2		
446	0221	0110	2784.3735	5.775E-02	5.27E-04	4.75E-04	-7.45E-05	-4.60E-06	0.00E+00	349	P58	2725.1365	R57	2825.1240	4		
448	0111	0000	2787.0168	1.890E-03	6.60E-05		-1.52E-05	0.00E+00		127	P41	2749.6913	R41	2814.7673	2		
447	0111	0000	2792.3683	3.705E-04	-2.48E-04		3.30E-05	0.00E+00		68	P25	2770.1756	R26	2811.9598	2		
446	0111	0000	2798.2926	1.020E+00	3.62E-04		-1.30E-06	0.00E+00		213	P70	2724.1891	R70	2840.9384	2	50	
446	1001	0110	2892.0513	2.800E-03	-5.46E-03		1.74E-05		3.10E-05	134	P46	2842.4297	R40	2917.1096	2		
446	1111	0200	2893.8473	1.400E-04				0.00E+00		9	Q11	2893.1904	Q19	2891.9636	1		
446	0510	0000	2897.8135	3.845E-04	5.32E-03		7.60E-06	0.00E+00		66	P19	2882.1770	R30	2924.5357	2		
446	1310	0000	3046.2129	1.780E-03	1.55E-02		3.29E-05	0.00E+00		121	P30	3019.9774	R48	3083.9421	2		
446	0002	1000	3132.4744	3.290E-03	5.04E-04		-2.50E-06			88	P43	3087.3271	R44	3159.2827	1		
446	2110	0000	3165.8536	3.395E-03	3.07E-02		-1.30E-06	0.00E+00		125	P22	3145.9640	R55	3202.6499	2		
456	0311	0110	3276.7317	3.590E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00		71	P24	3255.0958	R25	3297.1110	2		
456	0201	0000	3295.4621	3.340E-03	-1.10E-05		1.62E-05			90	P44	3253.9342	R45	3328.5019	1		
446	0531	0330	3302.1626	1.690E-03	0.00E+00		0.00E+00		0.00E+00	80	P39	3265.4105	R39	3331.3766	2		

Table 2. continued

<i>mol</i>	<i>band</i>	<i>band center</i>	<i>S<sub>V</sub></i>	<i>a<sub>1</sub>(e←e)</i>	<i>a<sub>1</sub>(f←f)</i>	<i>a<sub>2</sub>(e←e)</i>	<i>a<sub>2</sub>(f←f)</i>	<i>a<sub>3</sub>(f←e)</i>	<i>a<sub>3</sub>(e←f)</i>	<i>N</i>	<i>line</i>	<i>min. frq</i>	<i>line</i>	<i>max. frq.</i>	<i>N<sub>s</sub></i>	<i>NB</i>
446	0511	0310	3304.5216	1.410E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	146	P38	3268.4350	R38	3333.5421	2	
546	0311	0110	3311.4642	8.710E-04	1.36E-04	1.03E-03	0.00E+00	2.64E-05		129	P34	3280.6992	R36	3338.2309	2	
446	1311	1110	3320.5155	4.410E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00		88	P27	3295.8443	R28	3342.0525	2	
448	0311	0110	3320.9580	7.000E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00		118	P33	3291.7735	R33	3345.0582	2	
446	0421	0220	3321.9492	1.300E-02	2.34E-04	2.74E-04	2.53E-05	2.26E-05	0.00E+00	238	P52	3271.0980	R52	3359.3705	4	
446	0401	0200	3323.4098	1.840E-02	4.22E-04		1.62E-05			108	P53	3271.0085	R54	3360.3985	1	
546	0201	0000	3333.7393	9.460E-03	0.00E+00		0.00E+00			103	P51	3285.9791	R51	3368.6450	1	
446	0311	0110	3342.4797	1.835E-01	1.90E-04	1.99E-04	2.45E-05	2.47E-05	0.00E+00	312	P64	3276.8115	R65	3387.0280	4	6
448	0201	0000	3344.4035	8.270E-03	4.28E-04		3.50E-05			104	P51	3297.5547	R52	3378.8149	1	
446	1201	1000	3345.2578	5.450E-03	-3.30E-05		4.10E-05			97	P48	3299.3327	R48	3379.5875	1	
447	0201	0000	3354.0067	1.110E-03	0.00E+00		0.00E+00			70	P36	3321.5845	R37	3381.1233	1	
446	0201	0000	3363.9780	2.000E+00	1.84E-04		2.65E-05			148	P73	3288.5524	R74	3410.6822	1	68
446	0221	0000	3373.1414	1.780E-08	2.35E-04		-1.21E-05			111	P65	3310.2253	R66	3419.6696	1	
556	1001	0000	3394.1629	6.100E-04	-3.41E-03		6.80E-05			59	P35	3359.9509	R31	3414.8168	1	
456	2001	1000	3397.4437	1.000E-03	0.00E+00		0.00E+00			68	P35	3362.1222	R36	3421.0074	1	
546	2001	1000	3410.0262	5.000E-04	0.00E+00		0.00E+00			49	P29	3382.7269	R29	3429.7103	1	
446	1002	0001	3422.9834	1.730E-03	1.68E-03		-8.12E-05			75	P37	3385.2806	R39	3447.5832	1	
456	1111	0110	3423.1379	8.550E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	204	P49	3370.1232	R49	3452.1684	4	
448	1111	0110	3430.1069	4.328E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	189	P47	3383.3229	R47	3457.6795	4	
456	1001	0000	3432.1931	1.420E-01	0.00E+00		0.00E+00			126	P62	3360.8053	R63	3464.0792	1	
448	1001	0000	3434.9762	7.410E-02	0.00E+00		0.00E+00			124	P61	3369.7534	R62	3465.8351	1	
546	1111	0110	3436.9778	8.698E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	207	P50	3384.6477	R50	3465.6784	4	
446	2111	1110	3438.9080	7.603E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	204	P49	3386.2944	R49	3468.2692	4	
546	0600	0000	3443.6500	1.550E-01	0.00E+00		0.00E+00			12	P28	3418.0706	R26	3462.5776	1	
546	1001	0000	3443.6500	1.550E-01	0.00E+00		0.00E+00			129	P64	3372.0335	R64	3474.8659	1	
446	2001	1000	3445.9217	1.390E-01	0.00E+00		0.00E+00			126	P62	3375.0956	R63	3477.9987	1	
447	1111	0110	3451.6380	1.100E-03	0.00E+00	0.00E+00	0.00E+00			140	P36	3416.2799	R37	3475.6359	2	
446	1311	0310	3451.7160	7.550E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	201	P48	3399.9335	R49	3480.8263	4	
446	1331	0330	3455.5581	1.410E-02	0.00E+00		0.00E+00		0.00E+00	122	P52	3398.9676	R52	3486.0944	2	
447	1001	0000	3456.6363	1.530E-02	0.00E+00		0.00E+00			107	P53	3399.9744	R53	3485.7425	1	
446	1201	0200	3462.0289	1.330E-01	0.00E+00		0.00E+00			125	P62	3390.7569	R62	3494.0053	1	
446	1221	0220	3464.7175	1.290E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	308	P62	3393.9512	R62	3497.5485	4	
446	0600	0000	3466.5998	4.080E+01	8.00E-05		2.92E-06			22	P54	3425.0206	R52	3514.4731	1	1
446	0730	0110	3473.2117	1.000E-07	0.00E+00	0.00E+00	0.00E+00			6	P39	3433.4381	R37	3498.0316	2	
446	0710	0110	3473.2117	2.310E+00	0.00E+00		0.00E+00			4	P59	3406.8239	R58	3505.7387	1	
446	1111	0110	3473.2117	2.310E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	374	P73	3385.4778	R73	3507.4245	4	7
446	0620	0000	3474.4497	1.000E-07	0.00E+00		0.00E+00			33	P39	3445.8002	R40	3513.4770	1	
446	1001	0000	3480.8192	4.080E+01	8.00E-05		2.92E-06			166	P82	3378.0197	R79	3513.8631	1	40
448	1400	0000	3555.6771	8.300E-04	-4.60E-05		2.94E-05			65	P35	3527.2578	R35	3583.2610	1	
446	2001	0200	3562.6928	6.500E-04	2.11E-04		8.29E-05			62	P33	3526.8681	R34	3582.3480	1	
546	1400	0000	3589.9283	4.610E-04	0.00E+00		0.00E+00			47	P28	3567.0245	R28	3613.0965	1	
446	1600	0200	3599.0098	1.370E-03	0.00E+00		0.00E+00			75	P38	3565.6451	R38	3629.9773	1	
446	1510	0110	3609.1959	1.043E-02	2.60E-04	2.66E-04	3.36E-05	2.74E-05	0.00E+00	217	P51	3562.9261	R51	3652.8413	4	
446	1400	0000	3620.9431	9.800E-02	1.05E-04		1.89E-05			124	P61	3567.0072	R62	3670.1125	1	
446	2400	1000	3626.0922	7.180E-04	2.04E-03		0.00E+00			60	P31	3599.7567	R34	3654.5416	1	
446	1420	0000	3631.5897	1.830E-09	0.00E+00		0.00E+00			67	P51	3589.7271	R53	3677.7388	1	
448	2200	0000	3661.0237	4.120E-03	1.89E-04		1.04E-05			94	P46	3618.8302	R47	3692.2454	1	
456	2200	0000	3709.8128	1.250E-03	3.82E-04		7.20E-06			74	P37	3675.0632	R38	3737.9953	1	
546	2200	0000	3712.1285	3.350E-03	-3.90E-05		3.56E-05			92	P45	3670.5662	R46	3744.1824	1	
448	3000	0000	3735.3736	3.030E-03	1.70E-04		-2.21E-05			89	P44	3694.4405	R44	3764.1889	1	
446	3310	1110	3737.5034	3.910E-04	0.00E+00	0.00E+00	0.00E+00			76	P26	3713.6021	R26	3758.2714	2	
446	2510	0310	3740.5566	3.585E-04	0.00E+00	0.00E+00	0.00E+00			70	P24	3718.4261	R25	3760.5654	2	
446	3200	1000	3741.3996	7.240E-03	5.20E-05		3.16E-05			100	P49	3693.5715	R50	3775.9150	1	



Table 2. continued

<i>mol</i>	<i>band</i>		<i>band center</i>	<i>S<sub>V</sub></i>	<i>a<sub>1</sub>(e←e)</i>	<i>a<sub>1</sub>(f←f)</i>	<i>a<sub>2</sub>(e←e)</i>	<i>a<sub>2</sub>(f←f)</i>	<i>a<sub>3</sub>(f←e)</i>	<i>a<sub>3</sub>(e←f)</i>	<i>N</i>	<i>line</i>	<i>min. frq</i>	<i>line</i>	<i>max. frq.</i>	<i>N<sub>s</sub></i>	<i>NB</i>
446	2400	0200	3742.8633	5.060E-03	0.00E+00		0.00E+00				94	P46	3697.6468	R47	3775.4286	1	
446	2420	0220	3746.8438	3.230E-03	5.25E-04	-3.60E-05	3.63E-05	3.84E-05	0.00E+00	0.00E+00	186	P44	3704.5395	R45	3779.6340	4	
446	2310	0110	3747.0318	5.580E-02	2.00E-04	1.19E-04	2.04E-05	2.07E-05	0.00E+00	0.00E+00	272	P59	3686.2929	R59	3788.4984	4	
446	2200	0000	3748.2517	8.220E-01	1.27E-04		2.44E-05				141	P70	3675.6813	R70	3792.4630	1	
446	2220	0000	3766.0525	3.080E-09	3.38E-04		1.27E-05				82	P56	3713.6297	R58	3808.9537	1	
447	3000	0000	3781.6479	6.270E-04	0.00E+00		0.00E+00				56	P31	3752.6249	R32	3803.8562	1	
546	3000	0000	3795.4509	5.260E-03	4.46E-04		0.00E+00				96	P47	3748.5543	R48	3824.9898	1	
456	3000	0000	3816.4754	6.010E-03	0.00E+00		0.00E+00				96	P47	3765.4203	R48	3844.1541	1	
446	4000	1000	3820.7736	1.100E-02	1.95E-04		-2.30E-05				101	P50	3769.2910	R50	3852.6325	1	
446	0002	0110	3828.6099	2.095E-04	-1.53E-02		2.41E-04			0.00E+00	43	P33	3793.4995	R34	3828.6099	2	
456	3110	0110	3830.6951	2.920E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00			41	P21	3810.8329	R22	3846.9859	2	
446	3000	0000	3836.3710	1.800E+00	8.40E-05		-1.55E-05				144	P71	3754.0276	R72	3872.2899	1	61
446	4110	1110	3842.5580	5.055E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00			98	P29	3814.7975	R29	3864.2644	2	
446	3110	0110	3857.6146	8.300E-02	2.12E-04	6.70E-05	-1.29E-05	-1.48E-05	0.00E+00	0.00E+00	282	P60	3790.7304	R60	3893.1051	4	
446	3200	0200	3858.1706	3.740E-03	0.00E+00		0.00E+00				90	P44	3810.9106	R45	3884.8459	1	
446	3220	0220	3874.3628	4.060E-03	3.22E-04	0.00E+00	-1.75E-05	0.00E+00	0.00E+00	0.00E+00	191	P45	3827.9751	R45	3903.5201	4	
446	0311	0000	3931.2476	6.325E-04	-4.31E-03		1.30E-05		5.30E-06		93	P34	3899.6568	R29	3953.7841	2	
446	4000	0200	3937.5446	3.670E-04	2.14E-04		2.90E-05				38	P25	3912.4955	R26	3955.0917	1	
446	1201	0110	4041.3933	5.600E-04	-2.80E-03		8.55E-05			-6.20E-06	92	P34	4007.8870	R30	4062.9211	2	
446	1221	0110	4053.6943	7.502E-04	-4.53E-03	-4.80E-03	0.00E+00	0.00E+00	8.00E-07	3.00E-07	193	P35	4018.6001	R31	4076.3070	4	
446	1111	0000	4061.9796	1.370E-02	-4.54E-03		-3.20E-06		-1.60E-06		158	P54	4002.6625	R49	4091.1603	2	
446	2001	0110	4142.0572	1.890E-04	-1.11E-02		0.00E+00			4.60E-06	27	P21	4121.4963	Q38	4142.0572	2	
456	0112	0110	4299.6321	3.345E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00			62	P23	4276.9820	R24	4316.3230	2	
456	0002	0000	4326.6172	5.130E-03	-8.18E-04		0.00E+00				94	P47	4272.9040	R46	4350.9003	1	
446	1112	1110	4333.5512	2.885E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00			40	P19	4315.3038	R21	4348.4697	2	
446	2310	0000	4335.7996	1.715E-04	1.19E-02		3.36E-04		7.55E-06		32	Q 7	4335.7251	R26	4356.0620	2	
446	0222	0220	4360.6927	5.190E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	200	P46	4308.1102	R47	4385.0818	4	
446	0202	0200	4361.5627	5.670E-03	0.00E+00		0.00E+00				95	P47	4307.5851	R47	4385.8818	1	
446	1002	1000	4361.8369	5.260E-03	0.00E+00		0.00E+00				95	P47	4307.6740	R47	4385.4862	1	
546	0002	0000	4373.6061	3.440E-03	-4.33E-04		7.42E-06				91	P45	4323.9111	R45	4396.2479	1	
446	0112	0110	4388.9298	8.590E-02	-4.08E-04	-4.23E-04	8.60E-06	7.91E-06	8.00E-06	8.00E-06	285	P61	4312.7987	R59	4414.1279	4	
448	0002	0000	4403.0276	4.050E-03	-2.58E-04		7.10E-06				94	P47	4351.9420	R46	4425.5720	1	
447	0002	0000	4409.9286	6.390E-04	-8.26E-04		3.39E-05				58	P33	4376.0666	R32	4429.2595	1	
446	0002	0000	4417.3778	1.470E+00	-4.98E-04		3.58E-06				144	P72	4322.0069	R59	4442.2292	1	68
446	3110	0000	4446.3825	3.160E-04	1.38E-02		3.08E-05		0.00E+00		57	Q 4	4446.3157	R33	4469.3453	2	
446	0511	0110	4464.8189	3.255E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00			58	P22	4445.1877	R23	4484.2043	2	
446	0401	0000	4491.5421	2.360E-03	9.53E-04		4.87E-05				85	P42	4452.9078	R44	4524.8766	1	
448	1201	0000	4572.4905	3.370E-04	3.42E-04		0.00E+00				31	P23	4552.1732	R24	4589.5214	1	
546	1201	0000	4585.6700	6.380E-04	8.17E-04		1.81E-05				57	P31	4556.7341	R33	4608.2280	1	
446	1401	0200	4594.2404	1.010E-03	6.85E-04		0.00E+00				68	P35	4559.4361	R36	4618.7929	1	
446	1421	0220	4594.8787	7.000E-04	6.42E-04	4.01E-04	2.12E-05	0.00E+00			116	P32	4563.6298	R33	4618.3039	2	
446	2201	1000	4603.2025	6.260E-04	4.18E-04		0.00E+00				56	P31	4573.2768	R32	4625.7856	1	
446	1311	0110	4612.0133	1.043E-02	5.73E-04	5.09E-04	1.88E-05	2.06E-05	1.95E-05	1.95E-05	224	P51	4558.9572	R51	4644.4538	4	
446	0910	0110	4612.0134	1.040E-02	5.73E-04		1.88E-05				1	P23	4612.0134	R47	4640.9396	1	
446	1201	0000	4630.1612	1.260E-01	5.57E-04		2.49E-05				126	P62	4561.5053	R63	4664.9873	1	
446	1221	0000	4642.4622	7.020E-10	-2.78E-04		2.03E-05				31	P41	4601.9587	R44	4672.3329	1	
448	2001	0000	4650.5428	1.010E-03	6.88E-04		0.00E+00				70	P36	4614.7209	R37	4671.9160	1	
456	2001	0000	4677.7979	3.090E-03	2.54E-04		0.00E+00				88	P43	4629.1423	R44	4700.9117	1	
546	2001	0000	4679.9182	3.320E-03	1.75E-04		-1.40E-05				89	P44	4632.2314	R44	4703.0486	1	
446	3001	1000	4689.9417	3.720E-03	3.59E-04		0.00E+00				90	P44	4640.9572	R45	4714.2016	1	
446	2201	0200	4719.9736	2.430E-03	0.00E+00		0.00E+00				83	P42	4672.7654	R42	4742.8215	1	
446	2221	0220	4727.6665	2.523E-03	8.50E-06	7.95E-05	-2.50E-05	-1.56E-05	-2.00E-05	-2.00E-05	171	P42	4681.3817	R42	4751.6075	4	
446	2111	0110	4730.4058	4.780E-02	2.08E-04	2.69E-04	-1.45E-05	-1.50E-05	-1.46E-05	-1.46E-05	264	P57	4661.3572	R58	4757.1274	4	

Table 2. continued

<i>mol</i>	<i>band</i>	<i>band center</i>	<i>S<sub>v</sub></i>	<i>a<sub>1</sub>(e←e)</i>	<i>a<sub>1</sub>(f←f)</i>	<i>a<sub>2</sub>(e←e)</i>	<i>a<sub>2</sub>(f←f)</i>	<i>a<sub>3</sub>(f←e)</i>	<i>a<sub>3</sub>(e←f)</i>	<i>N</i>	<i>line</i>	<i>min. frq</i>	<i>line</i>	<i>max. frq.</i>	<i>N<sub>s</sub></i>	<i>NB</i>
446	2001	0000	4730.8251	9.050E-01	1.97E-04		-9.08E-06			140	P69	4641.2682	R60	4755.9515	1	51
446	1600	0000	4767.1421	8.870E-04	9.34E-04		0.00E+00			66	P34	4738.4945	R35	4796.9680	1	
446	2510	0110	4900.8539	1.000E-03	1.38E-04	-4.06E-04	2.30E-05	2.11E-05		138	P36	4866.5637	R36	4929.5806	2	
446	2400	0000	4910.9956	1.070E-02	3.26E-04		3.24E-05			104	P51	4861.9198	R52	4947.9715	1	
446	0202	0110	4940.9271	2.690E-04	-1.51E-03		0.00E+00		0.00E+00	43	P22	4919.6981	R17	4953.9488	2	
446	0222	0110	4949.6695	2.793E-04	3.56E-04	-6.31E-04	0.00E+00	0.00E+00	0.00E+00	86	Q 5	4949.4713	R22	4965.3347	4	
446	0112	0000	4977.6977	4.690E-03	-3.20E-04		0.00E+00	0.00E+00		142	P46	4925.4381	R46	5001.9939	2	
446	4200	1000	5010.5443	6.300E-04	0.00E+00		0.00E+00			57	P31	4980.1542	R32	5032.5724	1	
446	3400	0200	5024.1383	2.920E-04	0.00E+00		0.00E+00			21	P20	5005.4391	R21	5040.0547	1	
446	3200	0000	5026.3029	6.040E-02	3.00E-04		2.21E-05			120	P59	4960.6531	R60	5059.1346	1	
446	3310	0110	5029.0005	3.410E-03					0.00E+00	2	Q 1	5028.9888	Q 2	5028.9652	1	
446	0621	0110	5029.0005	3.430E-03	2.52E-04		2.09E-05			4	P14	5016.3921	R12	5039.0242	1	
446	3310	0110	5029.0012	3.420E-03	2.52E-04		2.09E-05	0.00E+00		90	P44	4982.4878	R45	5056.4265	2	
446	0621	0110	5029.0019	3.410E-03		1.21E-04		1.80E-05		8	P20	5010.8021	R19	5044.3024	1	
446	3310	0110	5029.0019	3.410E-03		1.21E-04		1.80E-05		88	P44	4984.5313	R45	5058.9039	1	
446	3420	0220	5032.4668	3.610E-04	0.00E+00		0.00E+00			34	P24	5009.8470	R25	5051.1832	1	
456	4000	0000	5073.0671	2.540E-04	1.43E-03		-6.01E-05			5	P25	5073.0671	R17	5085.7142	1	
446	5000	1000	5088.4044	4.010E-04	3.56E-04		-3.85E-05			40	P25	5064.6507	R26	5107.2814	1	
446	4000	0000	5105.6769	6.280E-02	3.06E-04		-3.04E-05			117	P58	5038.4097	R58	5134.9241	1	
446	4110	0110	5134.0558	2.830E-03	4.04E-04	2.04E-04	-2.20E-05	-1.96E-05	0.00E+00	170	P42	5088.4591	R43	5160.7766	4	
446	0202	0000	5529.6950	1.070E-03	-1.67E-04		5.33E-05			71	P37	5490.8148	R37	5552.6871	1	
446	0711	0110	5625.0488	1.220E-03		-5.46E-04		0.00E+00		2	P30	5592.4673	R28	5641.9869	1	
446	1112	0110	5625.0491	1.225E-03	-6.50E-04	-5.46E-04	0.00E+00	0.00E+00		142	P37	5582.6861	R37	5644.3801	2	
446	1002	0000	5646.7402	2.150E-02	-4.88E-04		0.00E+00			109	P54	5576.7350	R47	5666.4477	1	
446	1401	0000	5762.3727	5.570E-04	4.14E-04		6.02E-05			56	P31	5732.9656	R32	5785.8032	1	
446	2311	0110	5873.3014	5.745E-04	5.08E-04	8.74E-04	0.00E+00	0.00E+00		107	P30	5842.4362	R31	5894.1422	2	
446	2201	0000	5888.1059	8.080E-03	4.81E-04		2.02E-05			100	P49	5832.5145	R50	5914.2369	1	
446	3001	0000	5974.8451	2.200E-02	4.91E-04		-2.11E-05			108	P53	5907.8694	R50	5995.6676	1	
446	3111	0110	5982.0003	1.050E-03	3.92E-04	2.26E-04	-1.78E-05	-1.17E-05		136	P35	5942.9607	R36	6002.2666	2	
446	3400	0000	6192.2706	1.060E-03	3.73E-04		3.65E-05			70	P36	6156.7397	R37	6217.6832	1	
446	4200	0000	6295.4476	3.560E-03	3.65E-04		1.23E-05			90	P44	6246.0296	R45	6319.5106	1	
446	5000	0000	6373.3077	1.640E-03	2.63E-04		-3.31E-05			76	P38	6332.3880	R39	6396.2066	1	
446	0113	0110	6538.2109	1.773E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	160	P40	6488.6242	R39	6554.9094	4	
446	0003	0000	6580.8537	2.980E-02	-2.50E-04		0.00E+00			113	P56	6502.1070	R39	6597.3180	1	
446	2002	0000	6868.5498	7.750E-04	0.00E+00		0.00E+00			61	P33	6829.9712	R33	6884.6794	1	
446	3201	0000	7137.1271	8.900E-04	0.00E+00		0.00E+00			66	P34	7099.5696	R35	7156.4535	1	
446	4001	0000	7214.6799	8.500E-04	0.00E+00		0.00E+00			64	P34	7175.7841	R34	7232.2743	1	
446	1003	0000	7782.6616	4.300E-03	-1.99E-04		-2.47E-05			91	P45	7720.9105	R33	7796.6331	1	

mol=molecule: 446=<sup>14</sup>N<sub>2</sub><sup>16</sup>O, 456=<sup>14</sup>N<sup>15</sup>N<sup>16</sup>O, 546=<sup>15</sup>N<sup>14</sup>N<sup>16</sup>O, 448=<sup>14</sup>N<sub>2</sub><sup>18</sup>O, 447=<sup>14</sup>N<sub>2</sub><sup>17</sup>O, 556=<sup>15</sup>N<sub>2</sub><sup>16</sup>O, 458=<sup>14</sup>N<sup>15</sup>N<sup>18</sup>O, 548=<sup>15</sup>N<sup>14</sup>N<sup>18</sup>O

band= upper vibrational state then lower state, state given as  $\nu_1\nu_2\ell\nu_3$

frq. =frequency in cm<sup>-1</sup>

The F-factor coefficients,  $a_1$  and  $a_2$  pertain to R- and P-branch transitions and  $a_3$  to Q-branch transitions.

Table 3. Perturbed transitions included in the SISAM.N2O and HITRAN compilations

<i>mol</i>	<i>band</i>	<i>perturbed transitions</i>	<i>frequency extent (cm<sup>-1</sup>)</i>	
446	0201 0000	P71-P77 R69-R75	1107.3436	1234.9262
446	0201 0110	Q70 R69-R70	577.7600	640.9757
446	0400 0000	P54-P68 R52-R66	2269.9169	2382.6162
446	0401 0200	P54-P59 R52-R60	1106.2126	1206.6201
446	0420 0000	P54-P61 R52-R62	2288.0017	2392.4523
446	0420e 0220e	P54-P58 R52-R58	1107.5705	1205.8823
446	0510e 0110e	P51-P60 R49-R59	2260.4746	2360.7989
446	0510f 0110f	P52-P60 R50-R60	2264.8570	2366.4882
446	0600 0000	P44-P54 R42-R52	3425.0206	3514.4731
546	0600 0000	P23-P28 R21-R26	3418.0706	3462.5776
446	0600 0200	P40-P50 R38-R50	2258.0392	2342.6418
446	0620 0000	P25-P39 R23-R40	3445.8002	3513.4770
446	0620e 0220e	P25-P43 R22-R42	2263.4100	2335.7432
446	0620 1000	P29 R27	2168.8448	2216.3800
446	0621e 0110e	P13-P14 R11-R12	5016.3921	5039.0242
446	0621f 0110f	P18-P20 R15-R19	5010.8021	5044.3024
446	0710f 0110f	P59 R56-R58	3406.8239	3505.7387
446	0711f 0110f	P30 R28	5592.4671	5641.9869
446	0730e 0110e	P36 R34	3436.5330	3495.9923
446	0730f 0110f	P38-P39 R36-R37	3433.4381	3498.0316
446	0910e 0110e	R47		4640.9396
446	1001 0000	P36-P59 P31-P28 R26-R29 R34-R57	3413.6934	3511.4597
456	1001 0000	P50-P55 R48-R53	3370.8244	3461.9340
546	1001 0000	P14-P33 R12-R31	3411.7033	3464.2898
448	1001 0000	P47-P54 R45-R52	3378.9483	3463.4079
447	1001 0000	P44-P49 R42-R47	3405.2012	3483.9437
446	1001 0001	P28-P46 R26-R46	1215.2504	1292.0642
446	1001 0110e	P36-P46 P28-P31 R26-R29 R34-R40	2842.4297	2917.1096
446	1001 0110f	Q27-Q30 Q35-Q48	2877.5454	2887.3804
446	1001 1000	P36-P59 P28-P31 R26-R29 R34-R57	2134.9555	2232.3178
456	1001 1000	R48-R49	2184.4692	2184.9656
546	1001 1000	P14-P33 R12-R31	2143.5942	2195.9748
448	1001 1000	P47-P48 R45-R49	2173.0119	2211.5650
446	1111 0000	P34-P38 R32-R36	4023.2032	4085.9805
446	1111e 0110e	P61-P73 P34-P38 R32-R36 R59-R73	3395.4778	3506.6611
446	1111e 0110f	Q33-Q37	3464.8998	3466.5770
446	1111 1000	P34-P38 R32-R36	2740.8940	2803.4095
446	1111e 1110e	P61-P62 P34-P38 R32-R36 R59-R63	2117.2200	2220.7893
446	1111f 0000	Q35-Q55	4049.4842	4056.8521
446	1111f 0110e	Q35-Q42	3465.5735	3467.8775
446	1111f 0110f	P36-P73 R34-R73	3385.9712	3507.4245
546	1111f 0110f	P44-P50 R42-R50	3384.8671	3465.6784
446	1111f 1000	Q35-Q43	2772.6922	2774.1554
446	1111f 1110f	P36-P62 R34-R63	2116.9997	2220.7942
446	1112e 0110e	P23-P30 R21-R28	5592.4818	5641.9082
446	1112e 1110e	R41		4348.4526
446	1112f 0110f	P25-P35 R23-R33	5585.6029	5643.4998
446	1201 0000	P40-P62 R38-R60	4561.5053	4664.2541
446	1201 0200	P40-P62 R38-R60	3390.7569	3493.6249
446	1201 1000	P40-P48 R38-R48	3299.3327	3379.5875
446	1201 1200	P40-P47 R38-R47	2121.6450	2200.2516
446	1311e 0110e	P39-P50 R37-R51	4558.4011	4642.2362
446	1311e 0310e	P39-P48 R37-R49	3399.9335	3480.4622
446	1311f 0110f	P49-P51 R47-R51	4558.9572	4644.4538
446	1311f 0310f	R47-R49	3480.1500	3480.8263
446	3310e 0110e	P6 -P23 R4 -R21	5007.1459	5044.8557
446	3310e 1110e	P8 -P23 R6 -R21	3716.5927	3754.1486
446	3310f 0110f	P8 -P28 R6 -R26	5002.4851	5048.6519
446	3310f 1110f	P8 -P25 R6 -R26	3715.1582	3758.2714
446	4001 0000	P32-P34 R30-R34	7175.7841	7232.2743

frequency extent pertains to the minimum to maximum frequencies but all transitions of that molecule(mol) and band that lie between may not be perturbed.

Table 4. Extract from SISAM.N2O

M	I	position	line not.	strength	lower energy	linewidth air	self	shift air	band	line	o-c	measured shift	air-broadening $\Delta$ shf	width	$\Delta$ width	
4	1	1202.10869	48	5.79E-04	1573.68765	.0681	.0790	-.00184	03101 01101	R 48						TOTH02
4	1	1202.11095	54	1.27E-05	2424.38166	.0669	.0780	-.00206	04201 02201	R 54	1.20					TOTH02
4	1	1202.13421	27	4.50E-04	316.67167	.0720	.0917	-.00106	02201 00001	R 27						TOTH02
4	3	1202.20878	49	2.79E-05	990.91859	.0679	.0790	-.00188	02001 00001	R 49						TOTH02
4	1	1202.41292	55	1.48E-05	2459.21122	.0667	.0776	-.00210	04001 02001	R 55	-2.60					TOTH02
4	1	1202.88108	29	2.64E-04	1647.78476	.0715	.0897	-.00114	12001 10001	R 29						TOTH02
4	1	1202.91068	-84	1.68E-05	2982.75543	.0575	.0685	-.00314	10001 00001	P 84						TOTH02
4	1	1892.64640	7	2.46E-04	612.28562	.0847	.1099	-.00098	12202 01102	R 7						TOTH02
4	1	1892.69099	7	2.49E-04	612.24127	.0847	.1099	-.00098	12201 01101	R 7						TOTH02
4	1	1892.69848	23	6.57E-05	820.09975	.0733	.0944	-.00158	12001 01101	R 23						TOTH02
4	1	1893.21478	18	1.26E-05	1311.71624	.0756	.0981	-.00139	13101 02001	R 18						TOTH02
4	1	1893.25070	15	3.76E-03	100.55250	.0774	.1010	-.00128	11101 00001	R 15	-1.90	1.00	.0872	.0080		TOTH02
4	1	1893.46030	8	2.52E-04	619.00477	.0836	.1080	-.00102	12202 01102	R 8						TOTH02
4	2	2130.00869	-48	3.37E-03	984.46980	.0683	.0790	-.00270	00011 00001	P 48	-2.30	.50	.0695	.0020		TOTH02
4	1	2130.03980	-39	2.41E-05	3127.40235	.0698	.0830	-.00236	12211 12201	P 39						TOTH02
4	1	2130.04980	-51	1.02E-04	2881.36505	.0677	.0790	-.00281	03311 03301	P 51						TOTH02
4	1	2130.05213	-39	2.41E-05	3127.28169	.0698	.0830	-.00236	12212 12202	P 39						TOTH02
4	1	2130.26755	-40	4.01E-05	3011.38513	.0696	.0825	-.00240	04011 04001	P 40						TOTH02
4	1	2259.98982	56	2.21E-01	1335.68840	.0665	.0777	-.00316	00011 00001	R 56	-4.36	.30	.0660	.0007		TOTH02
4	4	2260.40836	-45	1.03E-05	818.16775	.0688	.0807	-.00271	04001 00001	P 45						TOTH02
4	1	2260.42098	57	1.78E-01	1383.32515	.0662	.0773	-.00320	00011 00001	R 57	-4.15	.45	.0667	.0008		TOTH02
4	1	2260.84501	58	1.43E-01	1431.79293	.0660	.0776	-.00323	00011 00001	R 58	-4.17	.30	.0652	.0015		TOTH02
4	1	2261.29288	-46	1.06E-05	2074.86647	.0686	.0803	-.00275	06001 02001	P 46	-7.31					TOTH02
4	1	2261.67170	60	9.14E-02	1531.22060	.0654	.0765	-.00331	00011 00001	R 60	-3.66	.40	.0641	.0020		TOTH02
4	4	2261.84817	-43	1.38E-05	747.86655	.0691	.0818	-.00264	04001 00001	P 43						TOTH02
4	2	2262.04047	-20	1.00E-05	175.94126	.0751	.0974	-.00179	04001 00001	P 20						TOTH02
4	1	2262.07435	61	7.25E-02	1582.17998	.0652	.0759	-.00335	00011 00001	R 61						TOTH02
4	2	3373.59446	-53	4.46E-05	1197.68164	.0673	.0776	-.00409	10011 00001	P 53	-2.35					TOTH02
4	1	3373.64674	11	3.79E-02	55.30638	.0805	.1040	-.00256	02011 00001	R 11	-2.07	.12	.0808	.0004		TOTH02
4	1	3373.71573	38	2.45E-05	1902.89675	.0698	.0830	-.00357	12011 10001	R 38	.03					TOTH02
4	4	3373.74653	-58	1.14E-05	1351.81332	.0662	.0773	-.00427	10011 00001	P 58						TOTH02
4	1	3373.97821	44	3.35E-04	1418.04093	.0688	.0807	-.00379	03111 01101	R 44						TOTH02
4	8	3374.06495	-22	1.19E-05	204.81738	.0741	.0961	-.00293	10011 00001	P 22						TOTH02
4	1	3430.20251	-47	3.25E-02	944.39240	.0685	.0790	-.00392	10011 00001	P 47	-25.87	-3.30	.30	.0704	.0006	TOTH02
4	1	3430.35953	-47	6.86E-03	944.39240	.0685	.0790	-.00392	06001 00001	P 47	25.16					TOTH02
4	3	3430.46178	-15	2.84E-03	97.15645	.0781	.1020	-.00273	10011 00001	P 15	.41					TOTH02
4	1	3430.49161	-41	5.70E-03	1310.06339	.0694	.0823	-.00369	11111 01101	P 41						TOTH02
4	2	3430.50677	-2	5.71E-04	2.51388	.0932	.1211	-.00225	10011 00001	P 2						TOTH02
4	1	3507.30600	43	7.98E-02	792.13835	.0690	.0810	-.00388	10011 00001	R 43	3.19	-4.35	.07	.0690	.0003	TOTH02
4	1	3507.67523	44	6.83E-02	828.95130	.0688	.0807	-.00392	10011 00001	R 44	7.22	-4.18	.16	.0691	.0004	TOTH02
4	1	3507.99683	45	4.82E-02	866.59809	.0686	.0803	-.00396	10011 00001	R 45	-25.87	-4.10	.10	.0684	.0003	TOTH02
4	1	3508.13143	35	1.11E-05	527.67426	.0703	.0851	-.00358	06201 00001	R 35	.01					TOTH02
4	1	3508.15384	45	1.02E-02	866.59809	.0686	.0803	-.00396	06001 00001	R 45	25.16	-1.50	.50	.0654	.0015	TOTH02
4	1	3508.36177	46	4.94E-02	905.07852	.0685	.0790	-.00399	10011 00001	R 46	-5.10	-4.52	.30	.0683	.0008	TOTH02
4	1	3508.69787	47	4.17E-02	944.39240	.0683	.0790	-.00403	10011 00001	R 47	-2.66	-4.68	.08	.0690	.0003	TOTH02
4	1	3509.02180	48	3.50E-02	984.53954	.0681	.0790	-.00407	10011 00001	R 48	-1.88	-3.98	.30	.0681	.0015	TOTH02
4	1	3509.04390	46	4.46E-04	905.07852	.0685	.0790	-.00399	06001 00001	R 46	3.13					TOTH02
4	1	3509.33502	49	2.93E-02	1025.51972	.0679	.0790	-.00411	10011 00001	R 49	-1.31	-4.42	.18	.0686	.0006	TOTH02
4	1	3509.63747	50	2.44E-02	1067.33274	.0677	.0790	-.00414	10011 00001	R 50	-1.01	-4.77	.24	.0677	.0006	TOTH02
4	1	5015.35111	-15	6.32E-05	689.36030	.0781	.1020	-.00426	33101 01101	P 15	-5.90					TOTH02
4	1	5015.57580	-15	6.36E-05	689.55030	.0781	.1020	-.00426	33102 01102	P 15	7.33					TOTH02
4	1	5015.63875	-12	1.07E-03	65.36143	.0805	.1040	-.00415	32001 00001	P 12						TOTH02
4	1	5016.31993	-14	4.69E-05	676.78737	.0789	.1030	-.00422	33101 01101	P 14	-17.76					TOTH02
4	1	5016.39209	-14	1.28E-05	676.78737	.0789	.1030	-.00422	06211 01101	P 14	54.40					TOTH02
4	1	5016.52530	-14	6.30E-05	676.95363	.0789	.1030	-.00422	33102 01102	P 14	5.78					TOTH02
4	1	5016.57815	-11	1.03E-03	55.30638	.0815	.1050	-.00411	32001 00001	P 11						TOTH02
4	1	5017.32003	-13	5.54E-05	665.05235	.0797	.1030	-.00419	33101 01101	P 13	11.80					TOTH02
4	1	5017.46687	-13	6.19E-05	665.19644	.0797	.1030	-.00419	33102 01102	P 13	4.22					TOTH02

M=molecule=4 for N<sub>2</sub>O. I=isotopic species, 1=<sup>14</sup>N<sub>2</sub><sup>16</sup>O, 2=<sup>14</sup>N<sup>15</sup>N<sup>16</sup>O, 3=<sup>15</sup>N<sup>14</sup>N<sup>16</sup>O, 4=<sup>14</sup>N<sub>2</sub><sup>18</sup>O, 5=<sup>14</sup>N<sub>2</sub><sup>17</sup>O, 6=<sup>14</sup>N<sup>15</sup>N<sup>18</sup>O, 7=<sup>15</sup>N<sup>14</sup>N<sup>18</sup>O, 8=<sup>15</sup>N<sub>2</sub><sup>16</sup>O

position is the computed position in cm<sup>-1</sup> unless o-c is given. o-c is observed minus computed position in cm<sup>-1</sup> × 10<sup>3</sup> and when o-c ≠ 0, position given is the observed value  
lower energy in cm<sup>-1</sup> and linewidth and shift values in cm<sup>-1</sup>/atm at 296K whereas the measured shift values and uncertainty,  $\Delta$ shf, in cm<sup>-1</sup>/atm. × 10<sup>3</sup>

band notation: upper vibrational state, lower vibrational state. Vibrational state given as  $\nu_1\nu_2\ell\nu_3$ . s is e for l and s is f for 2

line not. the notation is as follows: -x is Px, x is Rx, and 100+x is Qx.

strength in cm<sup>2</sup>/atm. at 296K and are computed unless transition is strongly perturbed in which case the observed value is given.

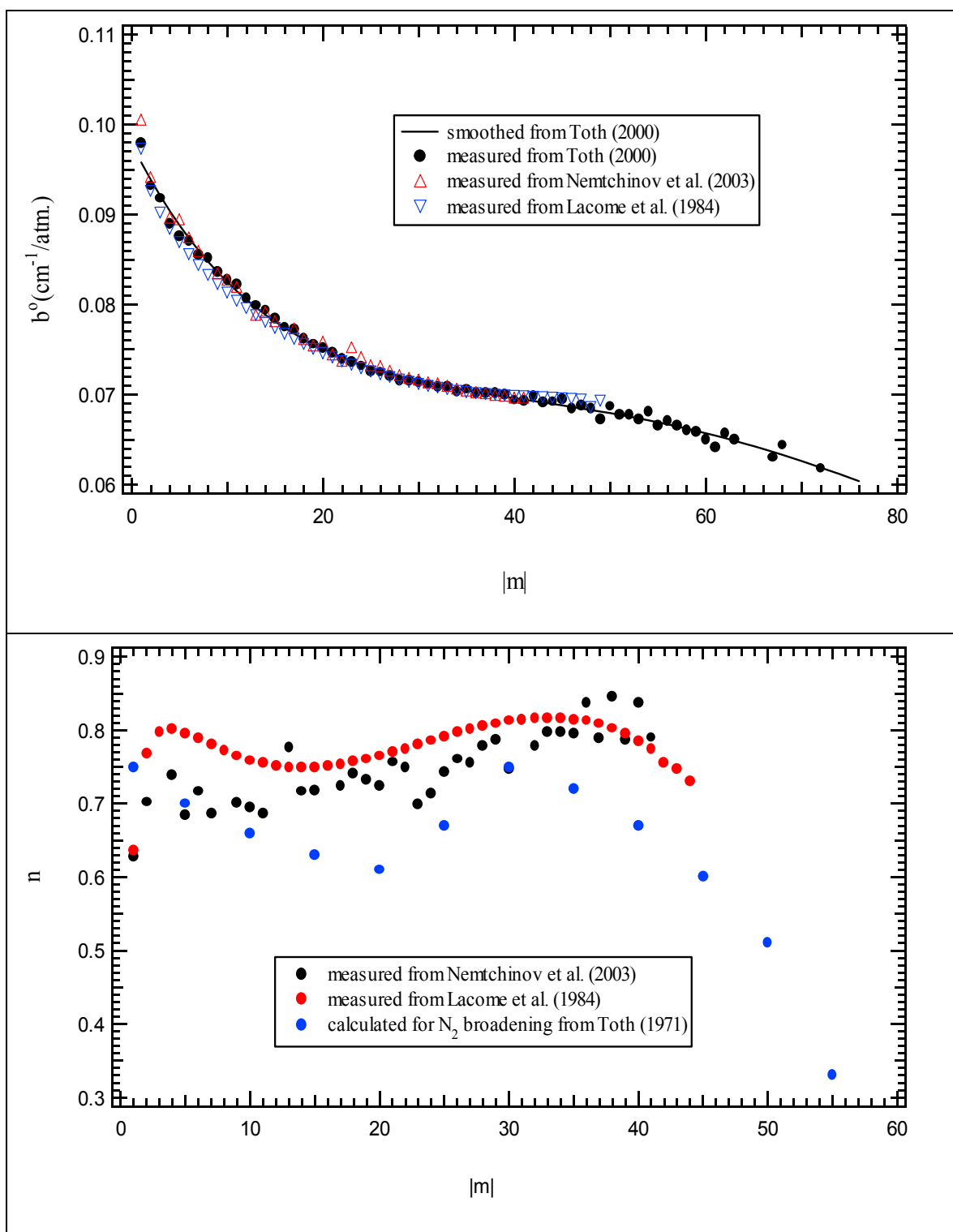


Figure 1. Linewidth coefficients,  $b^0$ , and temperature exponent,  $n$ , for air-broadening of  $\text{N}_2\text{O}$ .

$$b^0(T) = b^0(T^0)[T^0/T]^n$$

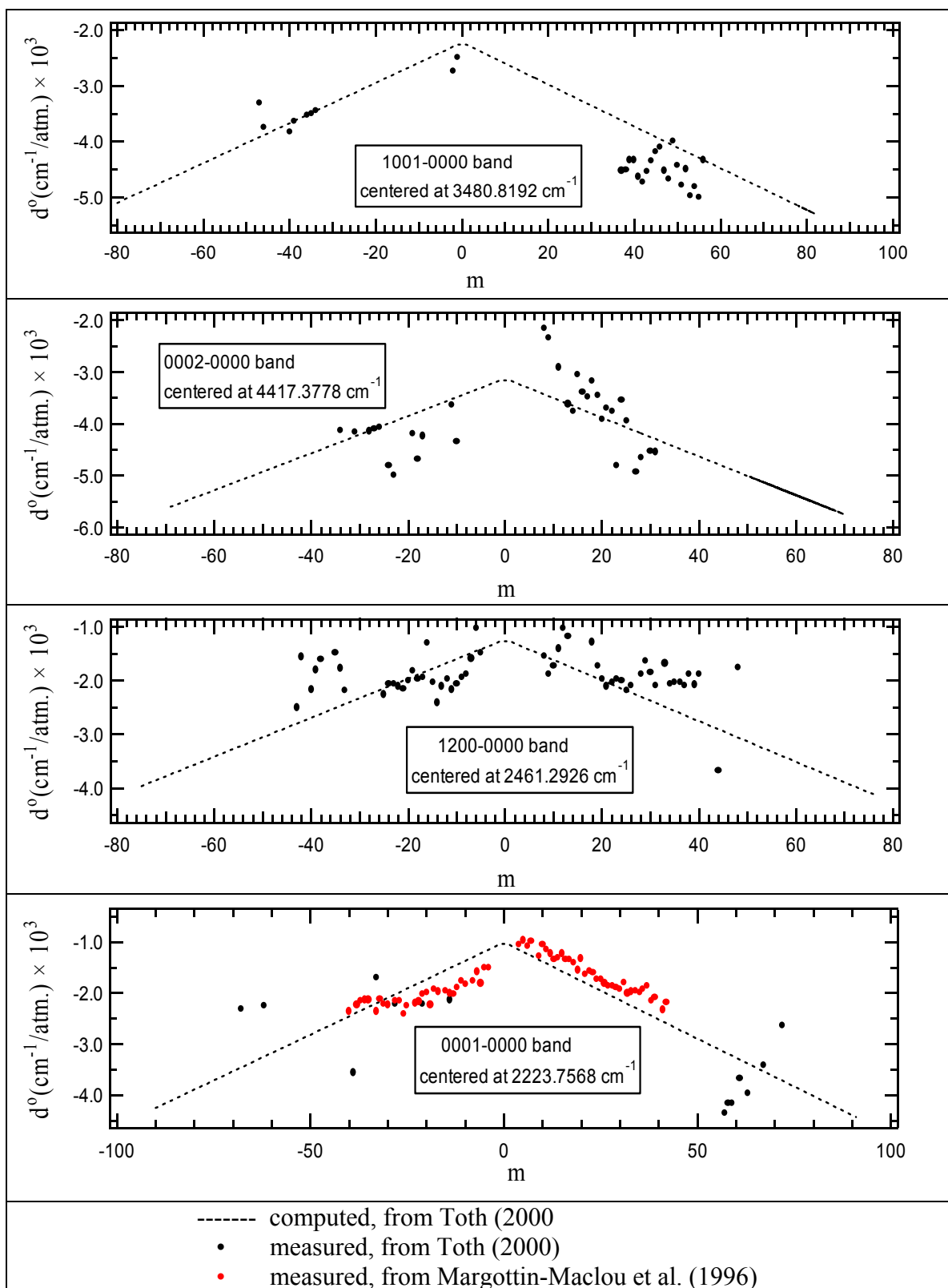


Figure 2. Pressure-induced frequency shift coefficients,  $d^0$ , of  $N_2O$  broadened by air at 296K