COMPILATION OF STRATOSPHERIC TRACE GAS
SPECTRAL PARAMETERS

TEXAS A AND M RESEARCH FOUNDATION

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Compilation of Stratospheric Trace Gas Spectral Parameters

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Atmospheric Transmittance
Infrared
Molecular Spectroscopy

This report describes a data compilation of the molecular spectroscopic parameters for a number of trace gases occurring in the stratosphere. The following molecules are included in the compilation: carbon monoxide, nitrous oxide, nitric oxide, nitrogen dioxide, sulfur dioxide and ammonia.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>DESCRIPTION OF THE COMPILATION</td>
<td>2</td>
</tr>
<tr>
<td>GENERAL REMARKS ON THE DERIVATION OF PARAMETERS</td>
<td>4</td>
</tr>
<tr>
<td>MOLECULAR SPECIES</td>
<td>4</td>
</tr>
<tr>
<td>BIBLIOGRAPHY FOR N&lt;sub&gt;2&lt;/sub&gt;O</td>
<td>21</td>
</tr>
<tr>
<td>BIBLIOGRAPHY FOR CO</td>
<td>29</td>
</tr>
<tr>
<td>BIBLIOGRAPHY FOR NO</td>
<td>37</td>
</tr>
<tr>
<td>BIBLIOGRAPHY FOR SO&lt;sub&gt;2&lt;/sub&gt;</td>
<td>43</td>
</tr>
<tr>
<td>BIBLIOGRAPHY FOR NO&lt;sub&gt;2&lt;/sub&gt;</td>
<td>49</td>
</tr>
<tr>
<td>BIBLIOGRAPHY FOR NH&lt;sub&gt;3&lt;/sub&gt;</td>
<td>52</td>
</tr>
<tr>
<td>BIBLIOGRAPHY FOR HNO&lt;sub&gt;3&lt;/sub&gt;</td>
<td>65</td>
</tr>
<tr>
<td>BIBLIOGRAPHY FOR OH</td>
<td>67</td>
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<td>BIBLIOGRAPHY FOR HCHO</td>
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COMPILATION OF STRATOSPHERIC TRACE GAS SPECTRAL PARAMETERS

INTRODUCTION

About three years ago, AFCRL provided a set of data, for the infrared region of the spectrum, for most of the naturally occurring molecules of significance in the terrestrial atmosphere. The following set of molecules (and their identification code) which were included in this first data compilation was: (1) water vapor; (2) carbon dioxide; (3) ozone; (4) nitrous oxide; (5) carbon monoxide; (6) methane; (7) oxygen. The present data compilation extends the previous work, by computing the pure rotation spectrum for molecules (4) nitrous oxide and (5) carbon monoxide. It also provides data on some pollutant gases for their strongest lines in the infrared region. These gases (and their identification code) are: (8) nitric oxide; (9) sulfur dioxide; (10) nitrogen dioxide; (11) ammonia; (12) nitric acid; (13) the hydroxyl radical; (14) formaldehyde. Table 1 gives the typical concentration of these trace gases in the terrestrial atmosphere.

TABLE 1. TYPICAL CONCENTRATION OF STRATOSPHERIC TRACE GASES IN DRY AIR

<table>
<thead>
<tr>
<th>Identification Number</th>
<th>Constituent</th>
<th>ppb by Volume</th>
<th>Reference</th>
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<tr>
<td>(4)</td>
<td>N\textsubscript{2}O</td>
<td>280</td>
<td>Birkland and Shaw, 1959</td>
</tr>
<tr>
<td>(5)</td>
<td>CO</td>
<td>75</td>
<td>Shaw, 1968</td>
</tr>
<tr>
<td>(8)</td>
<td>NO</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td>(9)</td>
<td>SO\textsubscript{2}</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>(10)</td>
<td>NO\textsubscript{2}</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>(11)</td>
<td>NH\textsubscript{3}</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>(12)</td>
<td>HNO\textsubscript{3}</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>(13)</td>
<td>OH</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(14)</td>
<td>H\textsubscript{2}CO</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
DESCRIPTION OF THE COMPILATION

The present compilation follows the same description as that given for Part 1 (AFCRL-TR-73-0096). The four essential parameters for each line are the line frequency, $v_o$ (cm$^{-1}$), the intensity per absorbing molecule, $S$ (cm$^{-1}$/molecule cm$^{-2}$), the Lorentz line width parameter, $a_o$ (cm$^{-1}$/atm), and the energy of the lower vibration-rotational state, $E^0$ (cm$^{-1}$). All of these quantities are given for a standard temperature, $T_s$, of 296$^0$K. The Lorentz line-width is usually assumed to vary in the way predicted by kinetic theory:

$$a_L = a_s(p/p_s)(T_s/T)^{1/2}$$

At very low pressures the lines assume a Doppler line-shape. This occurs when the parameter $a = (a_L/a_D) < 1.0$. Here $a_D$ is the width of a Doppler line at $1/e$ (where $e$ is the base of Naperian logarithms) of the maximum absorption of the line. It is given by

$$a_D = 4.298 \times 10^{-7} v_o (T/M)^{1/2}$$

where $M$ is the molecular weight of the absorbing gas. There is an intermediate regime when the line-shape is given by the Voigt line profile, which is simply the convolution of a Lorentz line profile and a Doppler line profile.

The line intensity, $S$, is independent of pressure but depends upon the temperature in the following way:

$$S(T) = S(T_s) \left( Q_v(T_s) Q_r(T_s) / Q_r(T) Q_v(T) \right) \exp \left[ \frac{1.439 E^0 (T - T_s)/T_s}{T} \right]$$

where $Q_v$ and $Q_r$ are the vibrational and rotational partition functions for the molecule. The temperature dependence of the rotational partition function is given by $(T/T_s)^{J}$ where $J$ is given in Table 2. The vibrational partition function is tabulated for some representative temperatures in Table 2.

In the past the line intensity has been defined in various units. We note that

$$1 \text{ (cm atm)}_{\text{stp}} = 2.69 \times 10^{19} \text{ molecules/cm}^2$$

and

$$1 \text{ (cm atm)}_{\text{room temperature (300$^0$K)}} = 2.45 \times 10^{19} \text{ molecules/cm}^2$$
TABLE I. VIBRATIONAL PARTITION FUNCTION

<table>
<thead>
<tr>
<th>Molecule</th>
<th>J</th>
<th>Temperature (°K)</th>
<th>175</th>
<th>200</th>
<th>225</th>
<th>250</th>
<th>275</th>
<th>296</th>
<th>325</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO</td>
<td>1.0</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td></td>
</tr>
<tr>
<td>NO$_2$</td>
<td>1.5</td>
<td>1.005</td>
<td>1.010</td>
<td>1.016</td>
<td>1.025</td>
<td>1.036</td>
<td>1.047</td>
<td>1.064</td>
<td></td>
</tr>
<tr>
<td>SO$_2$</td>
<td>1.5</td>
<td>1.014</td>
<td>1.025</td>
<td>1.038</td>
<td>1.055</td>
<td>1.074</td>
<td>1.093</td>
<td>1.121</td>
<td></td>
</tr>
<tr>
<td>NH$_3$</td>
<td>1.5</td>
<td>1.001</td>
<td>1.002</td>
<td>1.005</td>
<td>1.009</td>
<td>1.014</td>
<td>1.021</td>
<td>1.031</td>
<td></td>
</tr>
<tr>
<td>HNO$_3$</td>
<td>1.5</td>
<td>1.037</td>
<td>1.067</td>
<td>1.107</td>
<td>1.158</td>
<td>1.221</td>
<td>1.283</td>
<td>1.386</td>
<td></td>
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<tr>
<td>OH</td>
<td>1.0</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td></td>
</tr>
<tr>
<td>H$_2$CO</td>
<td>1.5</td>
<td>1.000</td>
<td>1.000</td>
<td>1.001</td>
<td>1.002</td>
<td>1.004</td>
<td>1.007</td>
<td>1.011</td>
<td></td>
</tr>
</tbody>
</table>

The same shorthand notation used in Part 1 has been adopted here to identify isotopic species. For example, $^{16}_0^{32}S^{16}_0 = 626$, etc. We have also used the same standard computer format for the data cards as was used in Part 1:

<table>
<thead>
<tr>
<th>$\nu$</th>
<th>S</th>
<th>$S_0$</th>
<th>$E''$</th>
<th>Rotation and Vibration ID</th>
<th>Date</th>
<th>Isotope</th>
<th>Molecule</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-10</td>
<td>11-20</td>
<td>21-25</td>
<td>26-35</td>
<td>36-70</td>
<td>71-73</td>
<td>74-77</td>
<td>78-80</td>
</tr>
<tr>
<td>F10.3</td>
<td>E10.3</td>
<td>F5.3</td>
<td>F10.3</td>
<td>5A6, A5</td>
<td>13</td>
<td>14</td>
<td>13</td>
</tr>
</tbody>
</table>

The numbers below each quantity refer to the columns on an IBM card, and the letter-number combinations represent the computer format. The first four quantities are $\nu$ = frequency in wavenumbers (cm$^{-1}$), $S$ = line intensity in cm$^{-1}$/molecules-cm$^{-2}$ at 296 °K, $a$ = halfwidth for Lorentz line shape, in cm$^{-1}$ at a pressure of 1 atm and a temperature of 296 °K, and $E''$ = energy of the lower state expressed in wavenumbers (cm$^{-1}$). As in Part 1, the rotation and vibration identifications are difficult to put in a standard format, due to differences in the number of quantum numbers required to specify lines in a particular band. (For example HNO$_3$ has nine fundamental modes of vibration, while NO has one, but it is split into two bands - one for the $^2\Pi_{1/2}$ state and one for the $^2\Pi_{3/2}$ state.) We have followed the formats used in Part 1, whenever it was possible. The remaining three fields specified above include the date the data were computed to be put on the tape, the isotopic code described above, and the identification number for the molecule given in Table 1.
GENERAL REMARKS ON THE DERIVATION OF PARAMETERS

The four tabulated parameters, \( v_0 \), \( E'' \), \( S \), and \( \alpha_0 \) must, of course, be derived from experimental observations. These observations are generally reproduced by a set of spectroscopic parameters and the quantum numbers for the line. In some cases the published data are poorly represented by the spectroscopic constants derived by the authors of these publications. Because this data compilation is intended for users interested in detecting pollutant molecules, perhaps by use of a laser, we have attempted to give line positions \((v_0)\) accurate to the Doppler (smallest) half-width of each line. The lower state energy levels have a similar accuracy. The line intensities should be accurate to ten percent and the line half-widths are of comparable accuracy. These details are discussed more fully in the following sections, where each of the molecules is described.

The parts of section 4 are numbered according to the identification number for each molecule and the missing parts have been described fully in Part 1 and this material will not be repeated here.

MOLECULAR SPECIES

Nitrous Oxide, Calculations by L.G. Young

The abundances of the isotopes used in computing the microwave (pure rotation) spectrum were taken from Part 1. The vibrational energy levels and the rotational constants associated with these levels were also taken from Part 1. Toth's measurements of nitrogen broadened half-widths were adopted, as in Part 1. A dipole moment of 0.166 Debye was adopted based on the microwave measurements of D.D. Coles, E.S. Elyash and J.G. Gorman (Phys. Rev. 72, 1265L), R.G. Shulman, B.P. Dailey and C.H. Townes (Phys. Rev. 75, 472A) and S.S. Tetenbaum (Phys. Rev. 88, 772, 1952). The computed line intensities are accurate to three significant figures; the half-widths are accurate to two significant figures.
Carbon Monoxide, Calculations by L.G. Young

The data in Part 1 were again used to compute the pure rotation spectrum of CO, and the dipole moment $\mu_e = 1.22$ Debye (J.S. Muenter "Electric Dipole Moment of Carbon Monoxide", J. Mol. Spectry. 590-491, 1975) was used. As a check on our intensity calculations, they were compared with the calculations of S.A. Golden (J. Quant. Spectry. Radiat. Transfer, 2, 201-214, 1962), the agreement between the two sets of calculations was found to be quite good. The line frequencies were compared with those given by Krupenie for the pure rotational lines of $^{12}\text{C}^{16}\text{O}$ and its isotopes, and the agreement was again good. The same half-widths of the lines used for the fundamental band in Part 1, were used for the pure rotation spectrum. The computed line intensities are accurate to three significant figures; the half-widths are accurate to two significant figures.

Nitric Oxide, Calculations by L.G. Young

Line Positions - Published spectroscopic data give a poor fit to measured line positions, so new constants had to be derived for this band. The effective rotational constants were obtained by fitting Keck's measurements of line positions in the $P$ and $R$ branches of the fundamental by a 6-th order polynomial in $m$:

$$\omega_i(m) = \omega_0 + a_i m + b_i m^2 + c_i m^3 + d_i m^4 + e_i m^5 + f_i m^6,$$

where the index $m = -J''$ for the $P$ branch and $m = J'' + 1$ for the $R$ branch. The coefficients in the polynomial are given by James and Thibault (eq.12) in terms of the effective rotational constants. Table 3 gives a comparison of the present rotational constants and previously published values.

The line positions and lower state energies of the fundamental band for the $^{14}\text{N}_{16}\text{O}$ isotope were calculated from the expression (eq.2 of James and Thibault)

$$E_{v_1}(J) = -\frac{3}{4} B_v - \frac{25}{16} D_v (-)^i \frac{1}{2} \delta_v + B_{v_1} J(J + 1) - D_{v_1} J^2(J + 1)^2 + H_{v_1} J^3(J + 1)^3,$$

where the subscript $v$ refers to the vibrational state and the subscript $i = 1$ refers to the $^2\Pi_{1/2}$ state; $i = 2$ refers to the $^2\Pi_{3/2}$ state. The
<table>
<thead>
<tr>
<th></th>
<th>present results</th>
<th>Keck</th>
<th>James and Microwave Thibault</th>
<th>Hall and Dowling</th>
<th>Palik and Rao</th>
<th>Meyer et al.</th>
<th>Olman et al.</th>
<th>Shaw</th>
</tr>
</thead>
<tbody>
<tr>
<td>$B_{01}$</td>
<td>1.672252 ± 0.000030</td>
<td>1.672171</td>
<td>1.67232</td>
<td>1.6718614</td>
<td>1.671854 ± 0.000081</td>
<td>1.6720</td>
<td>1.67198 ± 0.00004</td>
<td>1.67233 ± 0.00019</td>
</tr>
<tr>
<td>$D_{01} \times 10^6$</td>
<td>1.316 ± 0.040</td>
<td>1.16 ± 0.11</td>
<td>1.51 ± 0.95</td>
<td>1.13 ± 0.30</td>
<td>0.34 ± 0.30</td>
<td>1.8 ± 0.30</td>
<td>1.2 ± 0.30</td>
<td>1.6 ± 0.30</td>
</tr>
<tr>
<td>$H_{01} \times 10^{10}$</td>
<td>-6.54 ± 0.16</td>
<td>-7.26 ± 0.51</td>
<td>-3.98 ± 12.0</td>
<td>...</td>
<td>-14.2 ± 2.9</td>
<td>...</td>
<td>...</td>
<td>...</td>
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<tr>
<td>$B_{02}$</td>
<td>1.719990 ± 0.000025</td>
<td>1.720020</td>
<td>1.72025</td>
<td>1.7202435</td>
<td>1.720138 ± 0.000062</td>
<td>1.7198 ± 0.00012</td>
<td>1.71951 ± 0.00018</td>
<td>1.72012 ± 0.00018</td>
</tr>
<tr>
<td>$D_{02} \times 10^6$</td>
<td>9.721 ± 0.035</td>
<td>9.78 ± 0.12</td>
<td>10.33 ± 0.73</td>
<td>10.64 ± 0.23</td>
<td>10.24 ± 0.23</td>
<td>10.0 ± 0.23</td>
<td>9.7 ± 0.23</td>
<td>9.5 ± 0.23</td>
</tr>
<tr>
<td>$H_{02} \times 10^{10}$</td>
<td>7.02 ± 0.15</td>
<td>7.26 ± 0.51</td>
<td>11.1 ± 6.9</td>
<td>...</td>
<td>24.2 ± 2.1</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$B_{11}$</td>
<td>1.655140 ± 0.000030</td>
<td>1.655021</td>
<td>1.65524</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$D_{11} \times 10^6$</td>
<td>1.496 ± 0.040</td>
<td>1.27 ± 0.13</td>
<td>1.71 ± 0.95</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$H_{11} \times 10^{10}$</td>
<td>-6.12 ± 0.16</td>
<td>-7.07 ± 0.58</td>
<td>-3.71 ± 12.0</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$B_{12}$</td>
<td>1.701946 ± 0.000025</td>
<td>1.702053</td>
<td>1.70223</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
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</tr>
<tr>
<td>$D_{12} \times 10^6$</td>
<td>9.556 ± 0.035</td>
<td>9.71 ± 0.13</td>
<td>10.15 ± 0.73</td>
<td>...</td>
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<tr>
<td>$H_{12} \times 10^{10}$</td>
<td>6.48 ± 0.15</td>
<td>7.07 ± 0.58</td>
<td>10.1 ± 6.9</td>
<td>...</td>
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<td>...</td>
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<tr>
<td></td>
<td>present results</td>
<td>Keck</td>
<td>James and Microwave Thibault</td>
<td>Hall and Dowling</td>
<td>Palik and Rao</td>
<td>Meyer et al.</td>
<td>Olman et al.</td>
<td>Shaw</td>
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<td>----------------</td>
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<td>--------------</td>
<td>--------------</td>
<td>-----</td>
</tr>
<tr>
<td>$\omega_1$</td>
<td>1876.0909</td>
<td></td>
<td>1876.082</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>± 0.0007</td>
<td></td>
<td>0.0073</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\omega_2$</td>
<td>1875.8825</td>
<td></td>
<td>1875.874</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>± 0.0006</td>
<td></td>
<td>0.0062</td>
<td></td>
<td></td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>
molecular constants, $B_v$ and $D_v$, are obtained from the effective rotational constants, $B_{v1}$ and $D_{v1}$, by (eqs. 3 and 4 of Olman et al.)

\[
D_v = \frac{1}{2} (D_{v1} + D_{v2}) \text{ and}
\]

\[
B_v = \frac{1}{2} (B_{v1} + B_{v2} - D_v)
\]

The constant $\delta_v$ is related to the multiplet splitting parameter, $A_v$; James and Thibault (eq.4) give that relation. The value of Brown et al., $A_0 = 123.158 \text{ cm}^{-1}$, was used for the ground state. Lambda doubling causes the rotational energy levels to be split such that

\[
E_{\text{rot}} = E_{vi}(J) + E_{v1}^A(J)
\]

where

\[
E_{v1}^A(J) = - p(J + 1/2) + r_v(J - 1/2)(J + 1/2) (J + 3/2)
\]

and

\[
E_{v2}^A(J) = - r_v(J - 1/2)(J + 1/2) (J + 3/2)
\]

Here

\[
r_v = \frac{1}{\lambda_v - 2} \left[ 2q + \frac{P}{\lambda_v - 2} \right]
\]

where $p$ and $q$ are the A-doubling constants (Favero et al. give $p = 5.875 \times 10^{-3}$ and $2q = 7.68 \times 10^{-5} \text{ cm}^{-1}$) and $\lambda_v = A_v/B_v$.

The line positions, including A-doubling, were computed from

\[
\omega_i^P = \omega_i + \Delta^P + \delta_{i1} p
\]

\[
\omega_i^Q = \omega_i - \Delta^Q + \delta_{i1} 2p(J + 1/2)
\]

\[
\omega_i^R = \omega_i + \Delta^R - \delta_{i1} p
\]

where $\delta_{i1} = 0$ for $i \neq 1$ and $\delta_{i1} = 1$ for $i = 1$. The splitting common to both sub-bands is given by

\[
\Delta^P = (J - 1/2)(J + 1/2) \left[ 3/2(r_0 + r_1) + J(r_0 - r_1) \right],
\]

\[
\Delta^Q = (J - 1/2)(J + 1/2)(J + 3/2)(r_0 + r_1),
\]

and \[
\Delta^R = (J + 1/2)(J + 3/2) \left[ 5/2 r_0 + 1/2 r_1 + J(r_0 - r_1) \right].
\]
These calculated line positions differ slightly from those completed by Goldman et al., who fit Kecks data with a lower order polynomial in \( m \).

**Line Intensities** - A value of \( 128 \text{ cm}^{-1}/\text{cm-atm}_\text{stp} \) has been adopted for the band intensity of the most abundant (99.3%) isotope. Table 4 lists all the published measurements of the total band intensity. The early measurements which have subsequently been re-evaluated by the same author, and other values known to be inaccurate are indicated in parentheses; an inaccurately drawn value of the continuum was generally the source of error. The average of the 11 most recent measurements of the band intensity is \( 126 \text{ cm}^{-1}/\text{cm atm} \), when the values in parentheses are disregarded. When the measurements are weighted inversely with the square of the experimental error, then a value of \( 131 \text{ cm}^{-1}/\text{cm atm} \) is obtained. The band intensity reported by Varanasi and Penner lies between these two average values and is probably accurate to ten percent; that is our estimate of the error in the value adopted for these calculations.

In computing the line strengths, a pure Hund's case (a) was assumed. For this case, the line strengths are given by

\[
\begin{align*}
A_{P(J)} &= \frac{J^2 - \Omega^2}{J} \\
A_{Q(J)} &= \frac{(2J + 1)\Omega^2}{J(J + 1)} \\
A_{R(J)} &= \frac{(J + 1)^2 - \Omega^2}{J + 1}
\end{align*}
\]

A comparison of line intensities computed in this approximation with the line intensities calculated by James for intermediate coupling gave good agreement (within 3 percent) for all three branches at low values of \( J \). The discrepancies diminished with increasing \( J \) for the \( P \) and \( R \) branches, but increased in the \( Q \) branch (up to 10 percent by \( J = 41/2 \)); for this data compilation the inaccuracies in the \( Q \) branch is not serious since the line intensities rapidly diminish with increasing \( J \) (at \( J = 41/2 \) a line in the \( Q \) branch is at least 2 orders of magnitude weaker than corresponding lines in the \( P \) or \( R \) branches) and lines in the \( Q \) branch are unlikely to be used to detect NO as a pollutant gas.
<table>
<thead>
<tr>
<th>Intensity $\text{cm}^{-1}/\text{cm atm}_{\text{stp}}$</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>121 ± 6</td>
<td>Chandriah and Cho (1973)</td>
</tr>
<tr>
<td>135 ± 5</td>
<td>King and Crawford (1972)</td>
</tr>
<tr>
<td>134 ± 2</td>
<td>Michels (1971)</td>
</tr>
<tr>
<td>124 ± 22</td>
<td>Feinberg and Carmac (1967)</td>
</tr>
<tr>
<td>125 ± 8</td>
<td>Oppenheim, Aviv and Goldman (1967)</td>
</tr>
<tr>
<td>128 ± 10</td>
<td>Varanasi and Penner (1967)</td>
</tr>
<tr>
<td>122 ± 6</td>
<td>Abels and Shaw (1966)</td>
</tr>
<tr>
<td>132 ± 13</td>
<td>Alamichel (1966)</td>
</tr>
<tr>
<td>(103)</td>
<td>Jouve (1966)</td>
</tr>
<tr>
<td>115 ± 9</td>
<td>Ford and Shaw (1965)</td>
</tr>
<tr>
<td>(70)</td>
<td>Fukada (1965)</td>
</tr>
<tr>
<td>(76 ± 7)</td>
<td>Breeze and Torriso (1964)</td>
</tr>
<tr>
<td>138 ± 6</td>
<td>James (1964)</td>
</tr>
<tr>
<td>111 ± 7</td>
<td>Schurin and Cough (1963)</td>
</tr>
<tr>
<td>(82)</td>
<td>Vincent-Geisse (1954)</td>
</tr>
<tr>
<td>(70 ± 7)</td>
<td>Penner and Weber (1953)</td>
</tr>
<tr>
<td>(145 ± 29)</td>
<td>Insmore and Crawford (1949)</td>
</tr>
<tr>
<td>121</td>
<td>Havens (1938)</td>
</tr>
</tbody>
</table>
As an intermediate step in computing rotational line intensities, the rotational partition function was obtained by direct summation over states. At 296 °K, $Q_{\text{rot}} = 123.167062$ and $Q_{\text{rot}}^1 = 121.668583$; these values are slightly (less than 2 percent) larger than the rigid-rotor partition functions.

**Line Half-widths** - Abels and Shaw have measured self-broadened half-widths of the lines in both the $^2\Pi_{1/2}$ and $^2\Pi_{3/2}$ sub-bands and found "no significant difference either between the half-widths of lines with the same $|m|$ value in the R and P branches of the same sub-band or between corresponding lines of the two sub-bands." Their results agree within experimental error with the measurements of James, who also measured self-broadened linewidths. Ford reported that the self-broadening coefficient of NO, relative to $N_2$, was $1.00 \pm 0.05$ and this result was confirmed by Nachson and Coleman. (The fact that self-broadening is no more effective than foreign gas broadening was also demonstrated by Oppenheim, Aviv and Goldman, who used helium as the broadening gas). As a result of these measurements, we have assumed that air-broadened half-widths of NO will be identical to the half-widths measured by Abels and Shaw. It should be noted that Abels and DeBall have found that the line shape becomes super-Lorentzian for wavelengths greater than 1 cm$^{-1}$ from the line center.

Our tabulated half-widths were obtained from the linear fit to their data given by Abels and Shaw. Table 5 gives a comparison of half-widths measured for the fundamental with half-widths measured in the pure rotation spectrum and in overtone bands. The estimated error in the measurements for the fundamental band is 5 percent; the maximum spread in Abels and Shaw's data is 10 percent.
TABLE 5. COMPARISON OF HALF-WIDTHS MEASURED IN VARIOUS BANDS OF NO

<table>
<thead>
<tr>
<th>Rotational Line</th>
<th>Half-width</th>
<th>Reference</th>
<th>Rotational Line</th>
<th>Half-width</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 - 0 3/2</td>
<td>0.061</td>
<td>James</td>
<td>0 - 0 3/2</td>
<td>0.071</td>
<td>French and Arnold</td>
</tr>
<tr>
<td>1 - 0 3/2</td>
<td>0.063</td>
<td>Abels and Shaw</td>
<td>3 - 0 3/2</td>
<td>0.090</td>
<td>Meyer et al.</td>
</tr>
<tr>
<td>1 - 0 15/2</td>
<td>0.055</td>
<td>James</td>
<td>3 - 0 15/2</td>
<td>0.077</td>
<td>Meyer et al.</td>
</tr>
<tr>
<td>1 - 0 17/2</td>
<td>0.059</td>
<td>Abels and Shaw</td>
<td>2 - 0 17/2</td>
<td>0.081</td>
<td>Nachshon and Coleman</td>
</tr>
<tr>
<td>1 - 0 19/2</td>
<td>0.059</td>
<td>Abels and Shaw</td>
<td>2 - 0 19/2</td>
<td>0.070</td>
<td>Meyer et al.</td>
</tr>
<tr>
<td>1 - 0 29/2</td>
<td>0.052</td>
<td>James</td>
<td>2 - 0 29/2</td>
<td>0.059</td>
<td>Meyer et al.</td>
</tr>
<tr>
<td>1 - 0 37/2</td>
<td>0.050</td>
<td>Abels and Shaw</td>
<td>3 - 0 37/2</td>
<td>0.047</td>
<td>Meyer et al.</td>
</tr>
</tbody>
</table>

Nitrogen Dioxide, computed by D. Snider

Goldman et al. (1975) have computed the rigid rotor line intensities for the $v_3$ fundamental of $^{14}_N^{16}_O_2$. Their data compilation uses the spectroscopic constants derived by Hurlock, Lafferty and Rao (1974; see Table 6a) to fit their measurements of line positions for the $v_3$ fundamental. This is the strongest band of nitrogen dioxide; while it falls in the same spectral region (6.2 micron) as water vapor, it should be readily detectable at high resolution, particularly in the stratosphere. Goldman et al. have also computed data for the combination band $v_1 + v_3$ which is located at 3.4 microns, an atmospheric window region. For this weaker band, Goldman et al. used the spectroscopic constants derived by Olman and Hause (1968; see Table 6b). For both bands they used the integrated band intensity measured by Guttman: $S(v_3) = 2250 \text{ cm}^{-1}/\text{cm atm}_{\text{stp}}$ and $S(v_1 + v_3) = 69 \text{ cm}^{-1}/\text{cm atm}_{\text{stp}}$. Goldman et al. had measured the intensity of $v_3$ and found a somewhat lower value: $1640 \text{ cm}^{-1}/\text{cm atm}_{\text{stp}}$. The estimated accuracy of Guttman's value is ten percent, while the estimated accuracy of Goldman's value was twenty percent. Snider has recently revised the data for the $v_3$ band; he is currently revising the $v_1 + v_3$ band and is also doing $v_2$.

Tejwani computed half-widths for NO$_2$ broadened by nitrogen, $\gamma_{NO_2 - N_2}$ of $0.045 \text{ cm}^{-1}/\text{atm}$ and for NO$_2$ broadened by oxygen, $\gamma_{NO_2 - O_2}$ of $0.033 \text{ cm}^{-1}/\text{atm}$. He suggested that these values should be multiplied by factors...
of 1.4 and 1.2, respectively, to approximate the contribution of higher order terms which he neglected in his calculations. When this is done, we obtain a half-width for NO$_2$ broadened by air, $\gamma_{\text{NO}_2-\text{air}}$ of 0.058 cm$^{-1}$/atm. On the other hand, Goldman et al. assumed a half-width of 0.10 for their computed synthetic spectrum of the $v_3$ band. This suggests that the real value of the half-width is larger than the value obtained from Varanasi, so we have assumed a constant value for the half-width of 0.08 cm$^{-1}$/atm for this data compilation.

### TABLE 6a. GROUND STATE AND UPPER STATE CONSTANTS (IN UNITS OF cm$^{-1}$)

FOR THE $v_3$ BAND OF $^{14}$N$^{16}$O$_2$ CENTERED AT 1616.846 ± 0.0024 cm$^{-1}$

<table>
<thead>
<tr>
<th>Constant</th>
<th>000</th>
<th>001</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>8.002366 $\pm$ 0.000016</td>
<td>7.777200 $\pm$ 0.000742</td>
</tr>
<tr>
<td>$B$</td>
<td>0.4337050 $\pm$ 0.0000046</td>
<td>0.4309593 $\pm$ 0.0000123</td>
</tr>
<tr>
<td>$C$</td>
<td>0.4104482 $\pm$ 0.0000046</td>
<td>0.4078448 $\pm$ 0.0000115</td>
</tr>
<tr>
<td>$\Delta_{N}$</td>
<td>$(3.238 \pm 0.066) \times 10^{-7}$</td>
<td>$(3.263 \pm 0.030) \times 10^{-7}$</td>
</tr>
<tr>
<td>$\Delta_{NK}$</td>
<td>$(-1.943 \pm 0.016) \times 10^{-5}$</td>
<td>$(-2.254 \pm 0.010) \times 10^{-5}$</td>
</tr>
<tr>
<td>$\delta_{N}$</td>
<td>$(2.684 \pm 0.011) \times 10^{-3}$</td>
<td>$(2.744 \pm 0.062) \times 10^{-3}$</td>
</tr>
<tr>
<td>$\delta_{K}$</td>
<td>$(2.950 \pm 0.088) \times 10^{-8}$</td>
<td>$(3.556 \pm 0.268) \times 10^{-8}$</td>
</tr>
<tr>
<td>$H_{K}$</td>
<td>$(1.832 \pm 2.4) \times 10^{-6}$</td>
<td>$(-5.252 \pm 2.610) \times 10^{-6}$</td>
</tr>
<tr>
<td></td>
<td>$(2.04 \pm 0.532) \times 10^{-6}$</td>
<td>$(5.46 \pm 1.21) \times 10^{-6}$</td>
</tr>
</tbody>
</table>
TABLE 6b. CONSTANTS FOR THE $v_1 + v_3$ BAND OF $^{14}\text{N}^{16}\text{O}_2$ (IN UNITS OF cm$^{-1}$) WHICH IS CENTERED AT 2906.0737 ± cm$^{-1}$

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>$7.85404 \pm 0.0010$</td>
</tr>
<tr>
<td>B</td>
<td>$0.4285975 \pm 0.000017$</td>
</tr>
<tr>
<td>C</td>
<td>$0.4050070 \pm 0.000015$</td>
</tr>
<tr>
<td>$r_{aaaa}$</td>
<td>$(-1.1558 \pm 0.016) \times 10^{-2}$</td>
</tr>
<tr>
<td>$r_{bbbb}$</td>
<td>$(-1.4309 \pm 0.030) \times 10^{-6}$</td>
</tr>
<tr>
<td>$r_{aabb}$</td>
<td>$(7.469 \pm 0.17) \times 10^{-5}$</td>
</tr>
<tr>
<td>$r_{abab}$</td>
<td>$-8.214 \times 10^{-5}$</td>
</tr>
<tr>
<td>$H_{KN}$</td>
<td>$(-1.129 \pm 0.19) \times 10^{-7}$</td>
</tr>
<tr>
<td>$H_K$</td>
<td>$(2.893 \pm 0.04) \times 10^{-5}$</td>
</tr>
</tbody>
</table>

Sulfur Dioxide, Computed by D. Snider and S.A. Clough

The $v_3$ band, the strongest band of SO$_2$, is located near 7.3 microns and is overlapped strongly by the water vapor band at 6.3 microns. This fundamental band can only be used as a pollutant detector in the stratosphere. The $v_1$ band, which is only about ten percent as strong as the $v_3$ band, is much more suitably located, at 8.7 microns, for ground based measurements. It has also been suggested (Corice et al.) that the combination band $v_1 + v_3$, located at 4 microns, might be suitable for detecting sulfur dioxide in the telluric atmosphere. However, the combination band is nearly an order of magnitude weaker than the $v_1$ fundamental and its strength, as measured in the laboratory, is not well known (see Table 7). As a result, we have not included it in this data compilation. We have used Clough's calculations for the $v_1$ band and a band intensity of 104 cm$^{-1}$/cm atm stp. For the $v_3$ band we have used Snider's calculations of line positions and intensities but have adjusted the band origin by 0.029 cm$^{-1}$ to agree with the recent measurements of Dana and Fontinella of this band. Mayhood's band intensity was used for $v_3$. 

14
<table>
<thead>
<tr>
<th>Band Identification</th>
<th>Band Origin</th>
<th>Band Intensity $\text{cm}^{-1}/\text{cm atm}_{\text{std}}$</th>
<th>$\times 10^{20} \text{cm}^{-1}/\text{molecule cm}^{-2}$</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$v_1$</td>
<td>1151.71</td>
<td>93 ± 9</td>
<td>345 ± 35</td>
<td>Hinkley et al.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>106 ± 3</td>
<td>393 ± 10</td>
<td>Eggers and Schmid</td>
</tr>
<tr>
<td></td>
<td></td>
<td>117 ± 6</td>
<td>434 ± 25</td>
<td>Mayhood</td>
</tr>
<tr>
<td></td>
<td></td>
<td>96 ± 5</td>
<td>357 ± 20</td>
<td>Morcillo and Herranz</td>
</tr>
<tr>
<td></td>
<td></td>
<td>100 ± 5</td>
<td>371 ± 20</td>
<td>Burch et al.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>107 ± 6</td>
<td>397 ± 24</td>
<td>Tejwani et al.</td>
</tr>
<tr>
<td>average</td>
<td></td>
<td>103</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\sigma_{\text{int}}$</td>
<td></td>
<td>3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\sigma_{\text{int}}$</td>
<td></td>
<td>4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>weighted average</td>
<td></td>
<td>104</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$v_2$</td>
<td>517.75</td>
<td>116 ± 9</td>
<td>432 ± 43</td>
<td>Fox et al.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>125 ± 7</td>
<td>466 ± 25</td>
<td>Eggers and Schmid</td>
</tr>
<tr>
<td></td>
<td></td>
<td>120 ± 10</td>
<td>466 ± 37</td>
<td>Mayhood</td>
</tr>
<tr>
<td></td>
<td></td>
<td>125 ± 8</td>
<td>465 ± 29</td>
<td>Morcillo and Herranz</td>
</tr>
<tr>
<td>average</td>
<td></td>
<td>122</td>
<td></td>
<td>Tejwani et al.</td>
</tr>
<tr>
<td>$\sigma_{\text{int}}$</td>
<td></td>
<td>5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\sigma_{\text{ext}}$</td>
<td></td>
<td>2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>weighted average</td>
<td></td>
<td>123</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$v_3$</td>
<td>1362.0295</td>
<td>841 ± 84</td>
<td>3120 ± 300</td>
<td>Dana and Fontenella</td>
</tr>
<tr>
<td></td>
<td></td>
<td>845 ± 23</td>
<td>3170 ± 90</td>
<td>Eggers and Schmid</td>
</tr>
<tr>
<td></td>
<td></td>
<td>880 ± 27</td>
<td>3270 ± 100</td>
<td>Mayhood</td>
</tr>
<tr>
<td></td>
<td></td>
<td>815 ± 54</td>
<td>3020 ± 200</td>
<td>Morcillo and Herranz</td>
</tr>
<tr>
<td>average</td>
<td></td>
<td>848</td>
<td></td>
<td>Burch et al.</td>
</tr>
<tr>
<td>$\sigma_{\text{int}}$</td>
<td></td>
<td>31</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\sigma_{\text{ext}}$</td>
<td></td>
<td>14</td>
<td></td>
<td></td>
</tr>
<tr>
<td>weighted average</td>
<td></td>
<td>864</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Band Identification</td>
<td>Origin</td>
<td>Band Intensity cm(^{-1})/cm atm(_{\text{stp}}) (\times 10^{20}) cm(^{-1})/molecule cm(^2)</td>
<td>Reference</td>
<td></td>
</tr>
<tr>
<td>---------------------</td>
<td>--------</td>
<td>-------------------------------------------------</td>
<td>-----------</td>
<td></td>
</tr>
<tr>
<td>(v_1 + v_3)</td>
<td>2499.872 (\pm 0.003)</td>
<td>4.3 (\pm 0.3) 16 (\pm 1)</td>
<td>Barbe et al.</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>10 (\pm 2) 37 (\pm 7)</td>
<td>Secrun and Jouve</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>17.3 (\pm 3.5) 64 (\pm 13)</td>
<td>Chan and Tien</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>36.3 (\pm 0.3) 104 (\pm 10)</td>
<td>Burch et al.</td>
<td></td>
</tr>
<tr>
<td>average</td>
<td></td>
<td>17</td>
<td>Tejwani et al.</td>
<td></td>
</tr>
<tr>
<td>(\sigma_{\text{int}})</td>
<td></td>
<td>1.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\sigma_{\text{ext}})</td>
<td></td>
<td>7</td>
<td></td>
<td></td>
</tr>
<tr>
<td>weighted average</td>
<td></td>
<td>20</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 8 gives the Lorentz half-widths for SO\textsubscript{2} which were computed by Tejwani and measured by other investigators. There is quite a spread in the average values for the half-width, and we have arbitrarily chosen a value of $\gamma(296^\circ K)_{SO\textsubscript{2} - \text{air}} = 0.135\ \text{cm}^{-1}$.

TABLE 8. LORENTZ LINE HALF-WIDTHS FOR SULFUR DIOXIDE (cm\textsuperscript{-1})

<table>
<thead>
<tr>
<th>$\gamma_{SO\textsubscript{2}-SO\textsubscript{2}}$ at 300\textdegree K</th>
<th>$\gamma_{SO\textsubscript{2}-\text{air}}$ at 300\textdegree K</th>
<th>$\gamma_{SO\textsubscript{2}-\text{air}}$ at 250\textdegree K</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.27 - 0.58</td>
<td>0.079 - 0.129</td>
<td>Tejwani</td>
<td></td>
</tr>
<tr>
<td>0.13 - 0.45</td>
<td>0.083 - 0.125</td>
<td>Tejwani</td>
<td></td>
</tr>
<tr>
<td>0.304 - 0.431</td>
<td>0.15</td>
<td>Yang et al.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.076 - 0.129</td>
<td>Gebbie et al.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.152 + 0.015</td>
<td>Krishnaji et al.</td>
<td></td>
</tr>
<tr>
<td>0.500 + 0.075</td>
<td>0.152 + 0.015</td>
<td>Hinkley et al.</td>
<td></td>
</tr>
</tbody>
</table>

Ammonia, Computed By L.G. Young

The strongest band of NH\textsubscript{3} is the $\nu_2$ fundamental, located near 10.5 microns. The experimental results of Garing \textit{et al.} and Mould \textit{et al.} are poorly fit by the spectroscopic constants they obtained. The errors which result from using their constants to fit the line frequencies they measured are greater than 1 cm\textsuperscript{-1} for large values of the quantum numbers J and K (eg. J = K = 12). Taylor's (1973) calculations have this same fault: see Table 9. We have done a least squares fit to both sets of measurements and have obtained new constants for this band, which give better agreement with the observed line positions. We have used the band intensity measured by France and Williams, in computing the line intensity. Table 10 gives the published data for NH\textsubscript{3}. We have assumed a value of 0.09 cm\textsuperscript{-1} for the half-width.
TABLE 9. COMPARISON OF OBSERVED LINE POSITIONS FOR THE $v_2$ BAND OF AMMONIA AND THOSE PREDICTED USING THE ROTATIONAL CONSTANTS OF RAO et al.

<table>
<thead>
<tr>
<th>Line</th>
<th>Measured Line Position</th>
<th>Computed</th>
<th>Observed Minus Computed</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mould et al. (1959)</td>
<td>Garing et al. (1959)</td>
<td>Taylor (1973)</td>
</tr>
<tr>
<td>a(14,11)</td>
<td>-</td>
<td>648.20</td>
<td>648.328</td>
</tr>
<tr>
<td>a(14,10)</td>
<td>-</td>
<td>654.31</td>
<td>654.502</td>
</tr>
<tr>
<td>s(13,12)</td>
<td>-</td>
<td>655.46</td>
<td>655.525</td>
</tr>
<tr>
<td>s(15,14)</td>
<td>-</td>
<td>656.57</td>
<td>658.079</td>
</tr>
<tr>
<td>s(14,12)</td>
<td>-</td>
<td>680.86</td>
<td>680.925</td>
</tr>
<tr>
<td>s(14,11)</td>
<td>-</td>
<td>682.24</td>
<td>682.389</td>
</tr>
<tr>
<td>a(8,8)</td>
<td>1104.33</td>
<td>1104.33</td>
<td>1104.24</td>
</tr>
<tr>
<td>a(10,10)</td>
<td>1139.46</td>
<td>1139.45</td>
<td>1139.28</td>
</tr>
<tr>
<td>a(12,12)</td>
<td>1173.44</td>
<td>1173.46</td>
<td>1173.01</td>
</tr>
<tr>
<td>a(15,15)</td>
<td>1221.68</td>
<td>-</td>
<td>1220.94</td>
</tr>
<tr>
<td>a(15,10)</td>
<td>1245.81</td>
<td>-</td>
<td>1245.61</td>
</tr>
<tr>
<td>s(14,K)</td>
<td>1247.48</td>
<td>1247.50</td>
<td>1247.79</td>
</tr>
<tr>
<td>s(15,K)</td>
<td>1264.53</td>
<td>1264.51</td>
<td>1264.99</td>
</tr>
<tr>
<td>s(16,K)</td>
<td>1281.37</td>
<td>-</td>
<td>1281.98</td>
</tr>
</tbody>
</table>
### TABLE 10. INTENSITY AND HALF-WIDTH MEASUREMENTS FOR AMMONIA

<table>
<thead>
<tr>
<th>Band Center cm(^{-1})</th>
<th>Band Identification</th>
<th>Band Intensity (cm(^{-1})/cm atm(_{stpd}))</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>950 cm(^{-1})</td>
<td>(^{v}2)</td>
<td>790 ± 3</td>
<td>France and Williams</td>
</tr>
<tr>
<td></td>
<td></td>
<td>553 ± 110</td>
<td>McKean and Schatz</td>
</tr>
<tr>
<td>1628 cm(^{-1})</td>
<td>(^{v}4)</td>
<td>150 ± 5</td>
<td>France and Williams</td>
</tr>
<tr>
<td></td>
<td></td>
<td>67 ± 13</td>
<td>McKean and Schatz</td>
</tr>
<tr>
<td>3300 cm(^{-1})</td>
<td>(^{v}1), (^{v}3), and 2(^{v}4)</td>
<td>47 ± 3</td>
<td>France and Williams</td>
</tr>
<tr>
<td>3336 cm(^{-1})</td>
<td>(^{v}1)</td>
<td>20 ± 4</td>
<td>McKean and Schatz</td>
</tr>
<tr>
<td>3414 cm(^{-1})</td>
<td>(^{v}3)</td>
<td>13 ± 3</td>
<td>McKean and Schatz</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Half-width cm(^{-1})</th>
<th>(^{\gamma})NH(_3) - O(_2)</th>
<th>(^{\gamma})NH(_3) - N(_2)</th>
<th>(^{\gamma})NH(_3) - air</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0524</td>
<td>0.0925</td>
<td>0.0845</td>
<td></td>
<td>Legan et al.</td>
</tr>
<tr>
<td>0.0583</td>
<td>0.0963</td>
<td>0.0887</td>
<td></td>
<td>Smith and Howard</td>
</tr>
<tr>
<td>0.0470</td>
<td>0.0966</td>
<td>0.0867</td>
<td></td>
<td>Howard and Smith</td>
</tr>
<tr>
<td>0.0741</td>
<td>0.130</td>
<td>0.118</td>
<td></td>
<td>Bleany and Penrose</td>
</tr>
<tr>
<td>0.0510</td>
<td>--</td>
<td>--</td>
<td></td>
<td>Potter et al.</td>
</tr>
</tbody>
</table>

**Nitric Acid Vapor**

Snider and Goldman have made preliminary calculations for HNO\(_3\), but they do not feel that these are sufficiently accurate for our data tabulation.

**Hydroxyl Radical**

Benedict and Hall are making calculations for the strengths, energy levels and line positions based on Hall's solar spectrum. These calculations are not yet available, but they should be ready in a comparatively short span of time. They are using the Einstein A coefficients computed by Mies to calculate their line intensities.
Formaldehyde

The most extensive measurements of this vapor were made by Blau (1955). The two strong bands best suited for detecting \( \text{H}_2\text{CO} \) are \( v_4 \) at 2843 cm\(^{-1}\) and \( v_2 \) at 1746 cm\(^{-1}\). Unfortunately, I have been unable to find any measurements of band strengths for these fundamentals; as a result it is impossible to calculate absolute line intensities for this molecule in the infrared region of the spectrum.
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