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I. During this period the work on the spectral line parameters of the OH  $1^2\Sigma - X^2\Pi(0,0)$  band has been completed. A detailed paper describing this work has been published in J.Q.S.R.T. and a reprint is enclosed as an Appendix. Numerous reprint requests for this paper were received.

II. Using the methods developed for  $\text{NO}_2$  quantification (1) during previous phases of this project, the uv-visible data obtained during the 1977 balloon flights have been used for  $\text{O}_3$  quantification.

For atmospheric ozone amounts and the region covered by these spectra, the ozone absorption renders the atmosphere opaque at low sun angles in the 2800-3100Å region (Hartley bands). From about 3500 to 4000Å the ozone absorption coefficients are too small to give appreciable absorption even at the lowest sun angles scanned (~22°). From 4000 to 6000Å (Chappuis bands) the atmospheric absorption is quite weak and broad and does not have the contrast structure required for the three wavelengths method. The region from 3100Å to 3500Å appears to be the best region to use for determining ozone columns with the three-wavelength method.

Accurate determination of ozone columns and volume mixing ratios requires accurate ozone absorption coefficients measured at atmospheric temperatures (210 to 260K). The best presently available published absorption coefficients are those of Vigroux<sup>2</sup>. We have used these coefficients and five combinations of three wavelengths chosen from the features marked in Figure 1

to determine ozone columns and volume mixing ratios.

The ozone volume mixing ratios determined from the 9 February 1977 UV and 17 February 1977 UV data have been compared with standard middle-latitude ozone profiles<sup>3</sup>. The ozone profiles from both flights are in agreement with the standard profile mixing ratios, as shown in Figure 2.

The spectra in Fig. 1 have been smoothed to 2.5Å resolution. It should be noted that while the fine structure of the atmospheric O<sub>2</sub> absorption in Fig. 1 is not fully accounted for the Vigroux coefficients, it is in agreement with the recent high resolution (0.2Å) work being completed at the N.P.S.<sup>4</sup> The accuracy of the O<sub>2</sub> profiles should improve when this work, which is conducted at atmospheric temperatures, is completed.

III. Work has started on the new UV solar spectra obtained during the 3/19/81 balloon flight. Numerous high and low sun scans were obtained during ascent and from float altitude (~33 km) at 0.02Å resolution in the 3063-3099Å region. High and low sun scans from float altitude have been calibrated in wavelength. Representative scans are shown in Fig. 3 and Fig. 4 respectively for the 3070-3082Å region, which is considered best for OH measurements. The spectra are being studied for OH identification and quantification.

## REFERENCES

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9 FEB 77 RATIO OF SCAN 83 TO SCAN 56

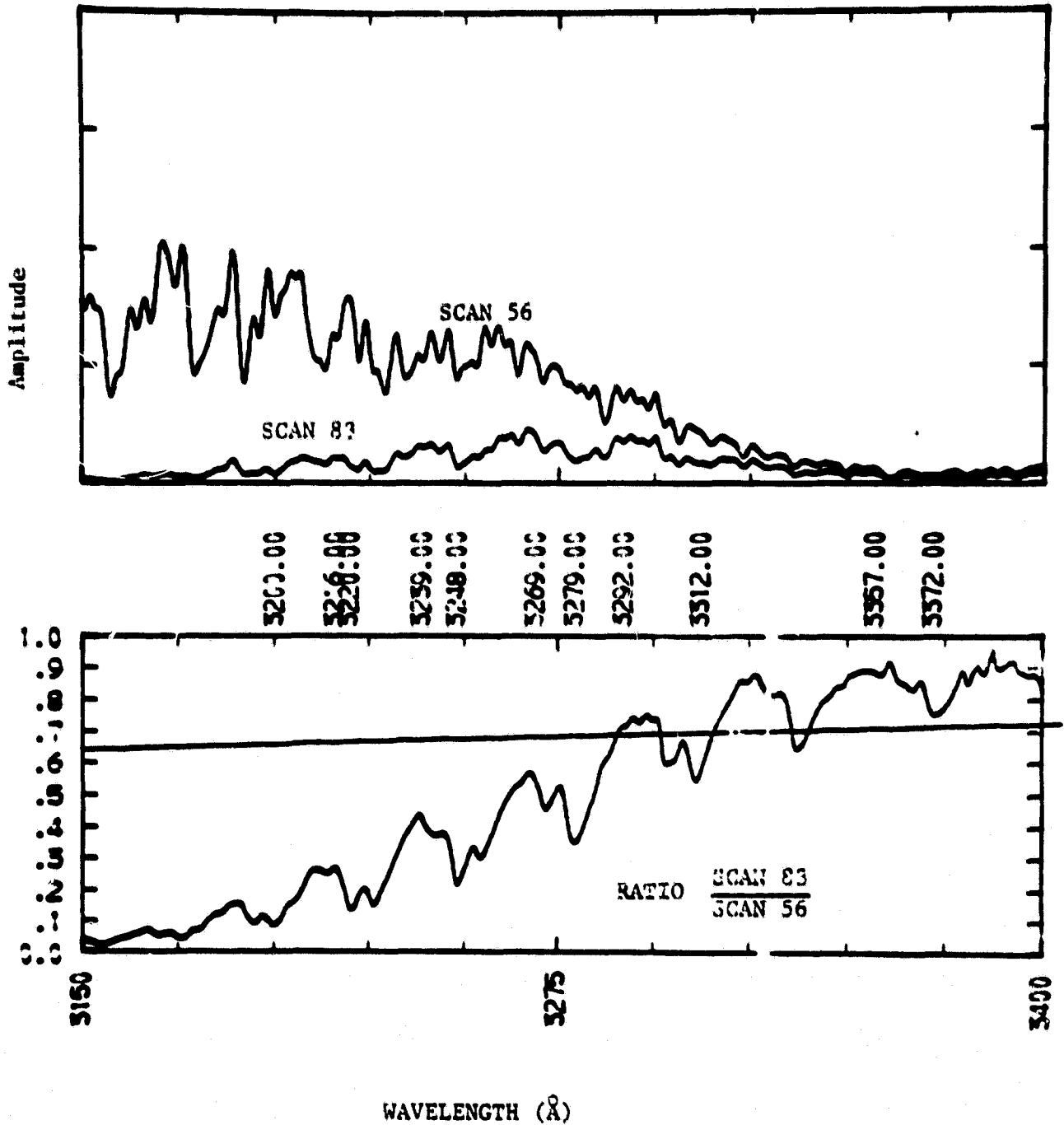


Fig. 1 Ratio of Scan 83 (low sun) to Scan 56 (high sun). The fine structure in the ratio spectrum is due to atmospheric O<sub>3</sub>. Resolution is 2.5Å.

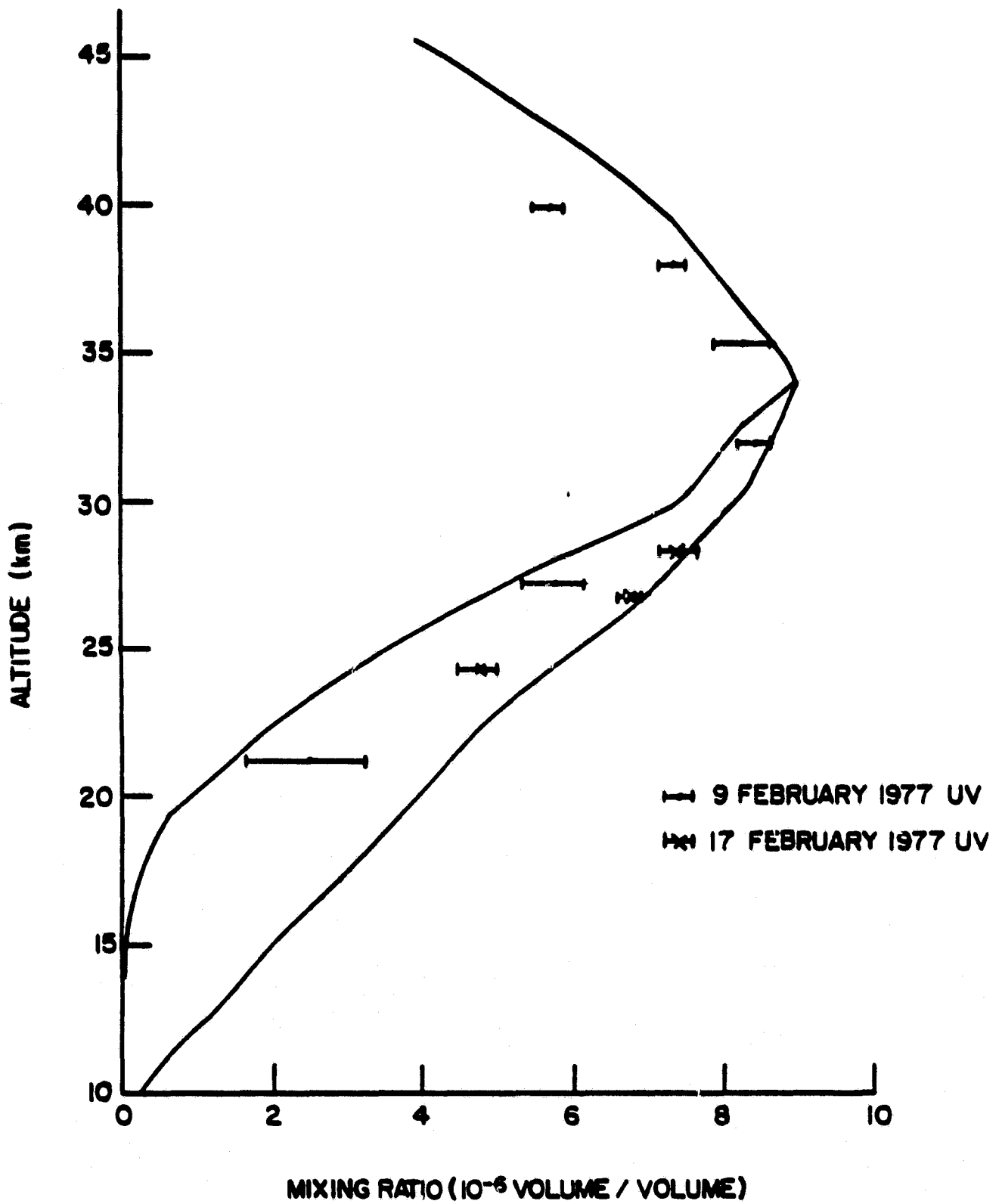


Figure 2 Preliminary ozone profiles superimposed on the standard midlatitude ozone profile of Mateer et al. (1980).

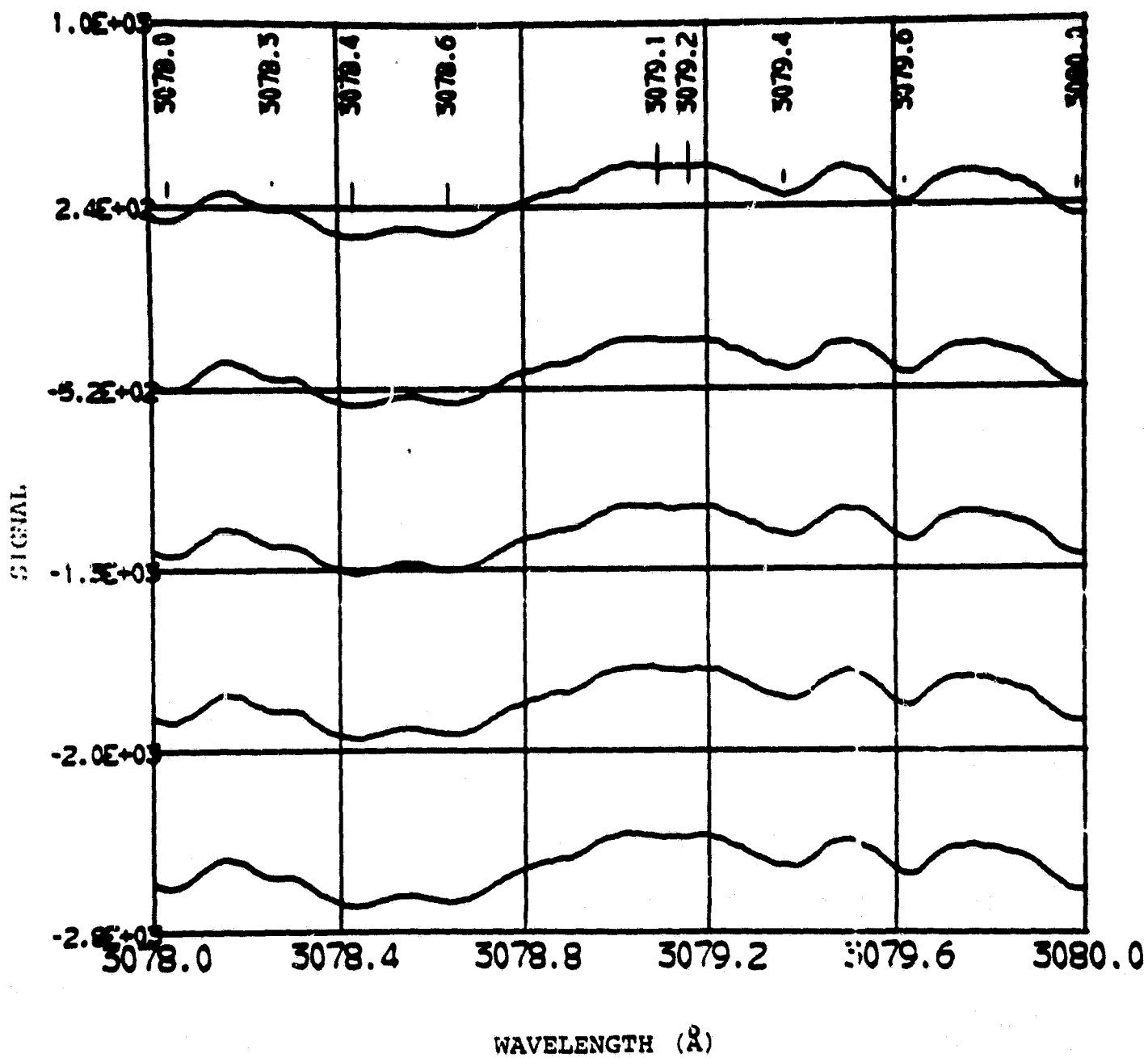


Fig. 3a Selected high sun scans obtained during the 3/19/81 balloon flight from float altitude (33 km). Resolution is 0.03Å.



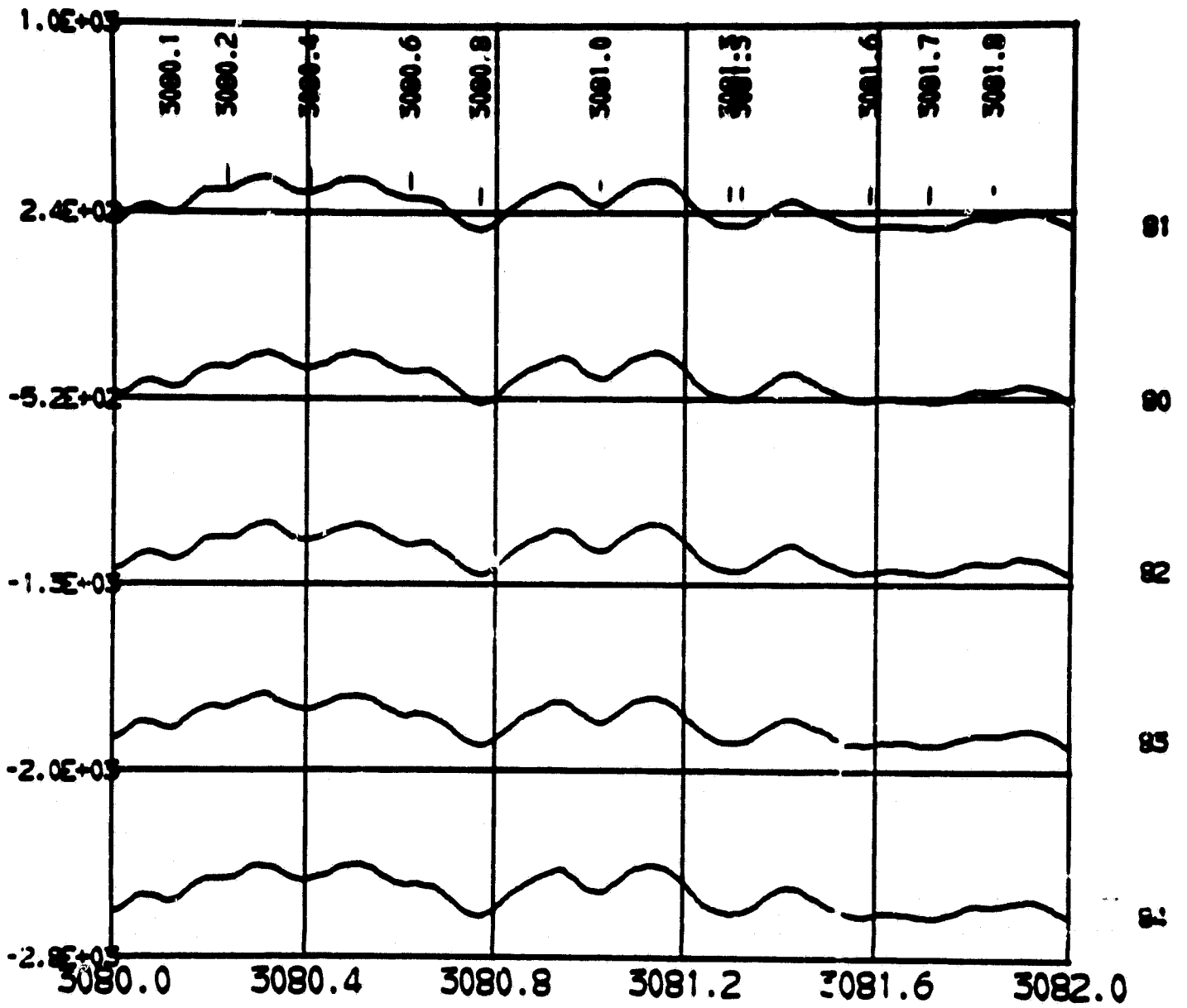


Fig. 3b

19 MAR 81 W57PT QUAR 1357

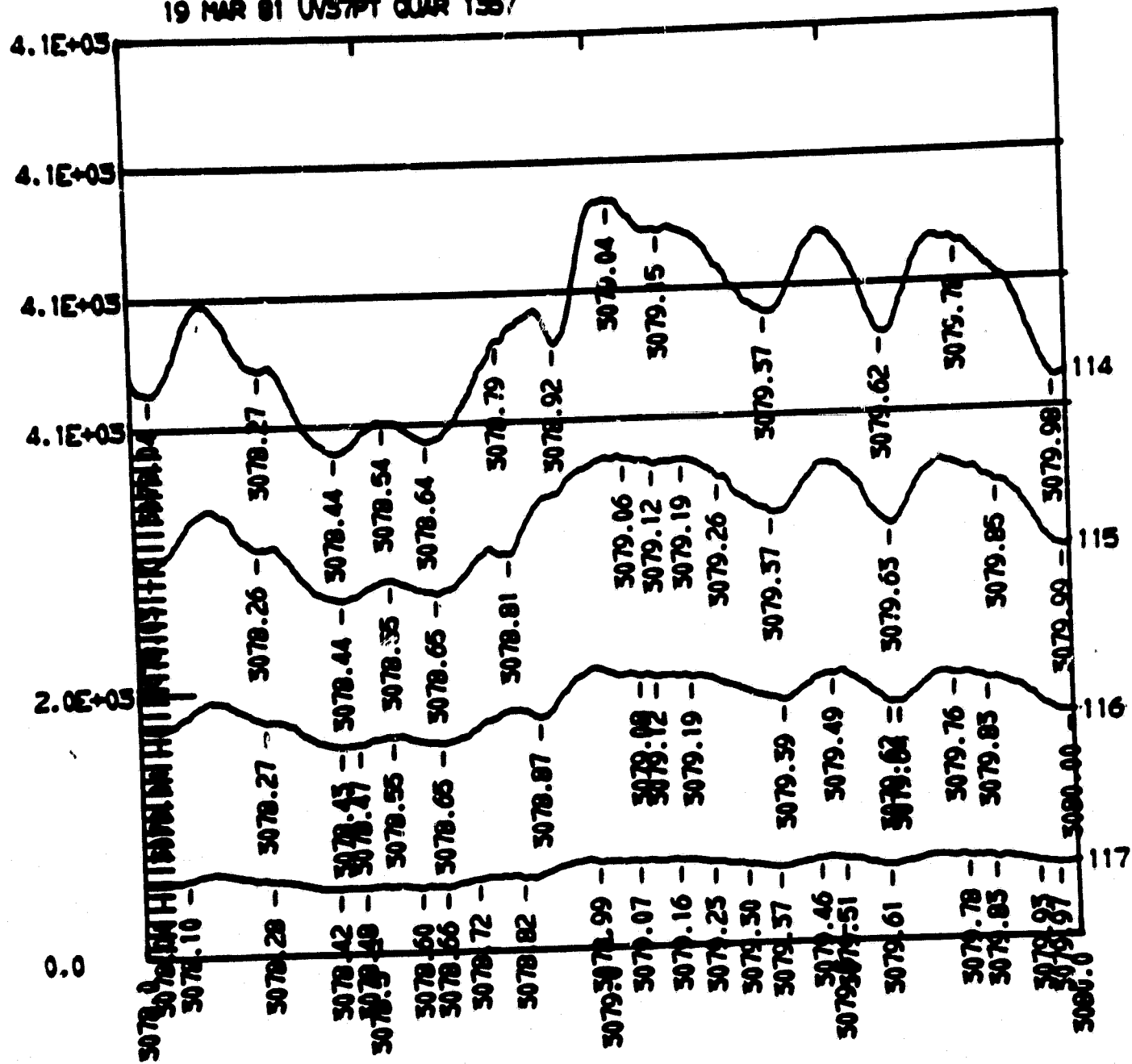


Fig. 4a Selected low sun scans obtained during the 3/19/81 balloon flight from float altitude (33 km). Resolution is 0.03Å.

19 MAR 81 UV57PT CLAR 157

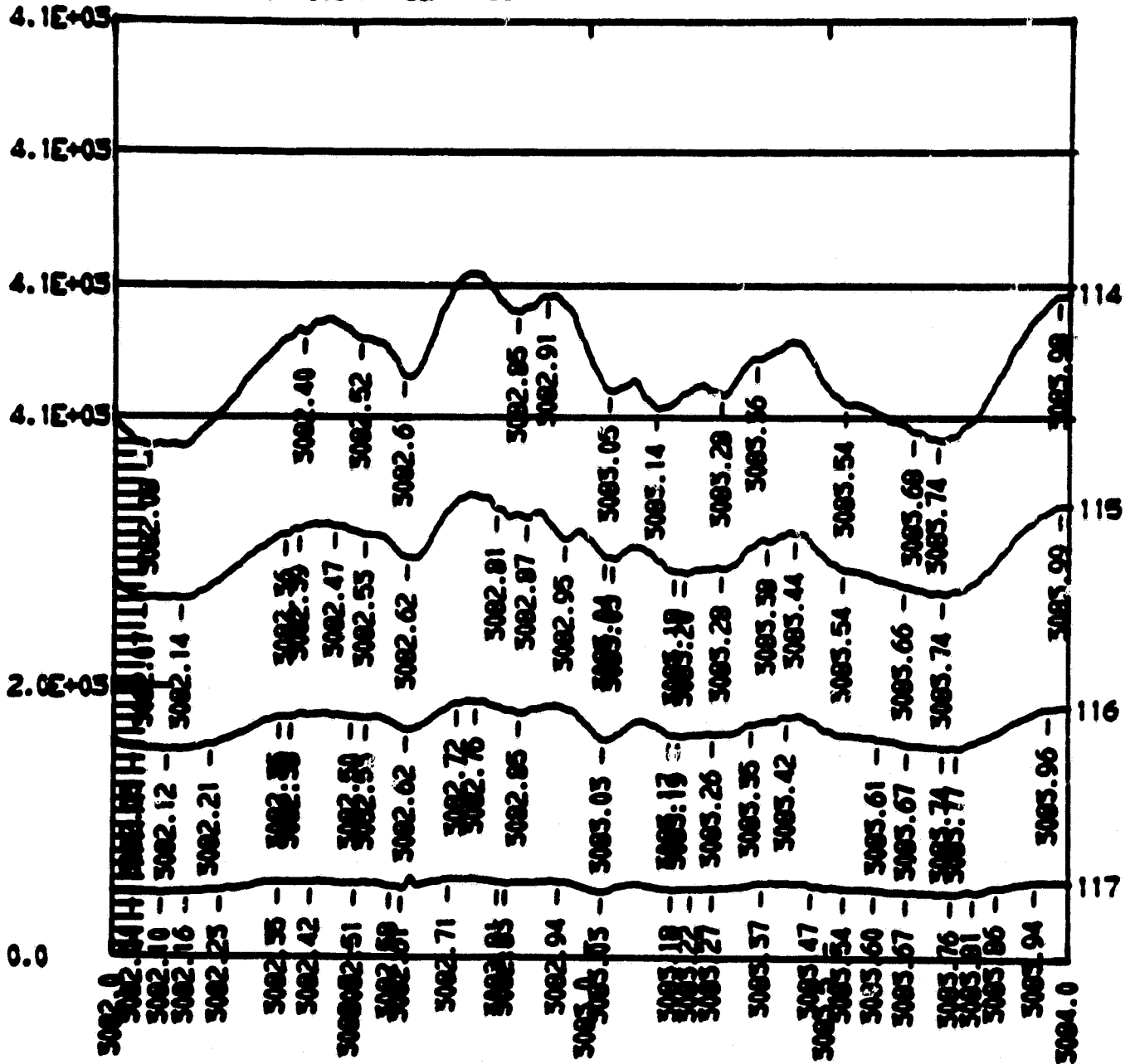


Fig. 4b

# SPECTRAL LINE PARAMETERS FOR THE $A^2\Sigma-X^2\Pi(0,0)$ BAND OF OH FOR ATMOSPHERIC AND HIGH TEMPERATURES

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**Abstract**—Individual spectral line parameters including line positions, strengths, and intensities, have been generated for the  $A^2\Sigma-X^2\Pi(0,0)$  band of OH, applicable to atmospheric and high temperatures. Energy levels and transition frequencies are calculated by numerically diagonalizing the Hamiltonian. Line strengths are calculated using the dipole matrix and eigenvectors derived from energy matrix diagonalization. The line strengths are compared to those calculated from previously published algebraic line strength formulas. Tables of line parameters are presented for 240 and 4600°K.

## 1. INTRODUCTION

The  $A^2\Sigma-X^2\Pi(0,0)$  band of OH in the 3005 Å region has been of interest to quantitative spectroscopists for many years because of its high absorption and emission intensity and convenient wavelength location for spectroscopic probes. The hydroxyl radical is a common by-product of most combustion processes, is present in atmospheric, solar and stellar spectra, and in recent years has been also recognized as an important trace constituent in atmospheric chemistry. Accurate determination of the amount of OH present during spectroscopic experiments depends on precise knowledge of line positions and intensities. Several analyses of spectral line positions for this band are available; among the more important of these are those of Dieke and Crosswhite,<sup>1</sup> who provided the first extensive analysis of the OH u.v. spectrum, and Destombes *et al.*,<sup>2</sup> who performed elaborate analysis of modern microwave, i.r. and u.v. OH data. Intensity (relative and absolute) studies of this band have been reviewed recently by Chidsey and Crosley,<sup>3</sup> who also performed extensive RKR calculations of rotational transition probabilities for the A-X system of OH.

The purpose of this work is to combine the best presently available data and theory to derive accurate quantitative line parameters for the  $A^2\Sigma-X^2\Pi(0,0)$  band, applicable to atmospheric and high temperatures. The results are displayed in line parameter tables, and include improved values for the line strength, calculated in intermediate coupling from the energy matrix eigenvectors.

## 2. LINE PARAMETERS DERIVATION

The OH molecule has an unpaired electron with total electronic angular momentum  $L = 1$  and  $S = 1/2$ . In the electronic ground state the projection of  $L$  along the internuclear axis is  $\Lambda = \pm 1$ . The projection of  $S$  along the internuclear axis is  $\Sigma = \pm 1/2$ , with a total electronic angular momentum projection  $\Omega = \Lambda + \Sigma$ . Here,  $\Lambda$ ,  $\Sigma$ ,  $\Omega$  are considered as signed quantities, as in the notation of Hougen.<sup>4</sup> The electronic ground state is an inverted  $^2\Pi$  state with the  $^2\Pi_{1/2}(\Omega = \pm 1/2, F_2)$  levels at higher energy than the  $^2\Pi_{3/2}$  levels ( $\Omega = \pm 3/2, F_1$ ). The rotational levels for this state are intermediate between Hund's cases (a) and (b). In the  $^2\Sigma$  upper state, which is Hund's case (b),  $\Lambda = 0$  and  $\Omega = \pm 1/2$  with  $J = N \pm 1/2$ . The  $^2\Pi$  and  $^2\Sigma$  states perturb one another and produce  $\Lambda$  doubling for each  $N$  ( $^2\Sigma_{1/2}$ ) or  $J$  ( $^2\Pi_{1/2,3/2}$ ).

We use the unique perturber approximation described by Destombes *et al.*<sup>2</sup> to calculate energy levels. This process is restricted to a single vibrational level  $v$  in the  $A^2\Sigma-X^2\Pi$  subspace. The total angular momentum number  $F$  (not to be confused with the level designations  $F_1$  and  $F_2$ ) is a good quantum number. For a given  $F$ , the  $J$  and  $J+1$  levels are weakly coupled by magnetic hyperfine interactions. These interactions are negligible in the calculation of electronic spectra and  $J$  may be considered a good quantum number. This procedure gives a  $6 \times 6$  Hamiltonian matrix, the elements of which are listed in Table 1. The matrix elements are

Table 1. Nonzero Hamiltonian matrix elements (Hund's case (a) basis).

| Matrix Elements   | Value   |
|---|---|
| $\langle {}^2\Pi_{1/2}   M   {}^2\Pi_{1/2} \rangle$       | $D_{\Pi}(n^2-2) + \frac{1}{2} - \frac{1}{2}n(n^2-3) + A_{\Pi}(n^2-2) + M_{\Pi}(n^2-3)n^2 + 3n^2 - 6$  |
| $\langle {}^2\Pi_{1/2}   M   {}^2\Pi_{3/2} \rangle$       | $D_{\Pi}n^2 - \frac{1}{2} - D_{\Pi}(n^2+n^2-1) - A_{\Pi}n^2 + M_{\Pi}(n^2+3)n^2 - 3n^2 + 2$   |
| $\langle {}^2\Pi_{1/2}   M   {}^2\Pi_{3/2} \rangle$       | $D_{\Pi}n - 2D_{\Pi}n(n^2-1) + M_{\Pi}n(3n^2-3n^2+3)$   |
| $\langle {}^2\Sigma_{1/2}   M   {}^2\Sigma_{1/2} \rangle$ | $D_{\Sigma}n^2 + \frac{1}{2} + \nu_0 - D_{\Sigma}(n^2+n^2) + M_{\Sigma}(n^2+3)n^2$  |
| $\langle {}^2\Sigma_{1/2}   M   {}^2\Sigma_{3/2} \rangle$ | $D_{\Sigma}n - 2D_{\Sigma}n^2 + M_{\Sigma}(3n^2+n^2)$   |
| $\langle {}^2\Pi_{3/2}   M   {}^2\Sigma_{1/2} \rangle$    | $\langle BL_{\Pi} \rangle n - \langle DL_{\Pi} \rangle n(2n^2-1) + \langle AL_{\Sigma} \rangle n + \langle ML_{\Sigma} \rangle n(3n^2+1)$   |
| $\langle {}^2\Pi_{3/2}   M   {}^2\Sigma_{-1/2} \rangle$   | $\langle BL_{\Pi} \rangle n - \langle DL_{\Pi} \rangle n(2n^2+1) + \langle ML_{\Sigma} \rangle n(3n^2+6n^2-2)$  |
| $\langle {}^2\Pi_{3/2}   M   {}^2\Sigma_{-1/2} \rangle$   | $-2\langle DL_{\Pi} \rangle n + \langle ML_{\Sigma} \rangle n(2n^2-1)n$   |
| $\langle {}^2\Pi_{3/2}   M   {}^2\Sigma_{1/2} \rangle$    | $\langle BL_{\Pi} \rangle n + \frac{1}{2} \langle AL_{\Sigma} \rangle + \langle DL_{\Pi} \rangle (6n^2-1) + \frac{1}{2} \langle AL_{\Sigma} \rangle (2n^2-1) + \langle ML_{\Sigma} \rangle (9n^2-3n^2+1)$ |

Notes:

$$1. \quad m = J \pm 1/2; \quad y = \{(J-1/2)(J+1/2)\}^{1/2}$$

2. Matrix elements are unchanged by exchange of initial and final states or by setting  $n$  to  $-n$  in both initial and final states.

written in Hund's case (a), with the wave functions represented by  $|\Lambda\Sigma\Sigma; J\Omega\rangle = |\Lambda\Sigma\Sigma; J\Omega\rangle$ , so that

$$\begin{aligned} {}^2\Sigma_{\pm 1/2}^+ &: |\Lambda\Sigma\Sigma; J\Omega\rangle = |0^+ 1/2 \pm 1/2; J \pm 1/2\rangle, \\ {}^2\Pi_{\pm 1/2} &: |\Lambda\Sigma\Sigma; J\Omega\rangle = |\pm 1 1/2 \pm 1/2; J \pm 1/2\rangle, \\ {}^2\Pi_{\pm 3/2} &: |\Lambda\Sigma\Sigma; J\Omega\rangle = |\pm 1 1/2 \pm 1/2; J \pm 3/2\rangle. \end{aligned} \quad (1)$$

The Hamiltonian constants used<sup>2</sup> are shown in Table 2 (these constants give a better fit to the

Table 2. Hamiltonian constants for  $A^2\Sigma-X^2\Pi(0,0)$ .

| Constant                            | Value <sup>a</sup><br>( $\text{cm}^{-1}$ ) |
|-------------------------------------|--|
| $B_{\Sigma}$                        | 16.9238973                                 |
| $D_{\Sigma}$                        | $2.0396602 \times 10^{-3}$                 |
| $M_{\Sigma}$                        | $97.7612 \times 10^{-3}$                   |
| $\nu_0$                             | $-7.8199 \times 10^{-3}$                   |
| $A$                                 | 32402.036230                               |
| $B_{\Pi}$                           | 18.3497336                                 |
| $D_{\Pi}$                           | $1.907952 \times 10^{-3}$                  |
| $M_{\Pi}$                           | $0.1239336 \times 10^{-6}$                 |
| $A_{\Pi}$                           | $-0.72330 \times 10^{-3}$                  |
| $\langle AL_{\Sigma} \rangle$       | -131.9226212                               |
| $\langle BL_{\Sigma} \rangle$       | 25.0435400                                 |
| $\langle DL_{\Sigma} \rangle$       | $2.6923336 \times 10^{-3}$                 |
| $\langle A_{\Pi}L_{\Sigma} \rangle$ | $8.651437 \times 10^{-3}$                  |
| $\langle ML_{\Sigma} \rangle$       | $0.166403 \times 10^{-6}$                  |

<sup>a</sup> Values are from Ref. 5 and are rounded to three figures beyond the standard errors indicated in Ref. 2.

observed spectrum than those of Ref. 2, which do not have a sufficient number of digits retained). The  $6 \times 6$  Hamiltonian matrix may be reduced to two  $3 \times 3$  blocks by the Kronig transformation.

$$|J\Omega\delta\rangle = \frac{1}{2}(|\Lambda S\Sigma\rangle|J\Omega\rangle + \delta|-\Lambda S-\Sigma\rangle|J-\Omega\rangle), \quad (2)$$

where  $\delta$  equals  $s = \text{symmetric} = +$  or  $a = \text{antisymmetric} = -$ . This notation should not be confused with the  $s, a$  and  $+, -$  notation for homonuclear diatomic molecules.<sup>†</sup> In this new basis, one of the  $3 \times 3$  blocks contains only matrix elements of the type  $\langle J'\Omega's|H|J\Omega s\rangle$  and the other contains only matrix elements of the type  $\langle J'\Omega'a|H|J\Omega a\rangle$ .

After numerical diagonalization of a  $3 \times 3$  Kronig transformed block, the electronic state of each eigenvalue (energy level or, more properly, term value in  $\text{cm}^{-1}$ ) may be determined by noting that the largest eigenvalue belongs to the  $^2\Sigma_{1/2}$  state, the intermediate eigenvalue to the  $^2\Pi_{1/2}$  state, and the smallest eigenvalue to the  $^2\Pi_{3/2}$  state. The remaining quantum numbers and parities may be determined from Table 3.

The selection rules for the  $A^2\Sigma-X^2\Pi(0,0)$  electric dipole allowed transitions are  $\Delta J = 0, \pm 1$ ,  $\Delta N = 0, \pm 1, \pm 2$ . Parity selection rules require  $+\leftrightarrow-, +\leftrightarrow+,$  and  $-\leftrightarrow-,$  which give for the wavefunction the Kronig symmetry selection rules of  $s \leftrightarrow s$  and  $a \leftrightarrow a$  for  $\Delta J = \pm 1$  ( $P$  and  $R$  branches) and  $s \leftrightarrow a$  for  $\Delta J = 0$  ( $Q$  branches). Transitions are designated by  ${}^{\Delta N}\Delta J_{F''}(J')$  where ' refers to the upper state and '' refers to the lower state and  $F$  is  $F_1$  or  $F_2$ . These selection rules permit 12 branches, of which 6 are main branches ( ${}^F P_{11}, {}^Q Q_{11}, {}^R R_{11}, {}^F P_{22}, {}^Q Q_{22}, {}^R R_{22}$ ) and 6 are (weaker) satellite branches ( ${}^Q P_{21}, {}^R Q_{21}, {}^S R_{21}, {}^Q Q_{12}, {}^Q R_{12}, {}^O P_{12}$ ).

The line intensities  $S_{lu}(T)$  ( $\text{cm}^{-1}/\text{atm-cm}$ ) at temperature  $T$  ( $^{\circ}\text{K}$ ) are calculated from<sup>6</sup>

$$S_{lu}(T) = \frac{1}{8\pi c\nu^2} \left(\frac{N}{p}\right) \frac{e^{-1.4388E''/T}}{Q_{vR}} A_{21}^{j'j''} (2J'+1)(1 - e^{-1.4388\nu T}), \quad (3)$$

where  $\nu (= E' - E'')$  is the transition frequency in  $\text{cm}^{-1}$ ,  $c = 2.99792458 \times 10^{10}$   $\text{cm}/\text{sec}$ ,  $N$  is the total number of OH molecules/ $\text{cm}^3$ ,  $p$  is the pressure in atm,  $A_{21}^{j'j''}$  is the Einstein  $A$  coefficient in  $\text{sec}^{-1}$ ,  $E''$  is the lower state energy ( $= E_l$ ), and  $Q_{vR}$  is the vibration rotation partition function.

Line intensities may be converted from  $\text{cm}^{-1}/\text{atm-cm}$  at  $T$  to  $\text{cm}/\text{molecule}$  at  $T$  by

$$S_{lu}(T)(\text{cm}/\text{molecule}) = 3.721963 \times 10^{-20} \frac{T(^{\circ}\text{K})}{273.16(^{\circ}\text{K})} S_{lu}(T)(\text{cm}^{-1}/\text{cm-atm}). \quad (4)$$

The  $S_{lu}(T)$  in  $\text{cm}/\text{molecule}$  are at the population temperature.

We assume that  $Q_{vR}$  is given by  $Q_v Q_R$ , where the vibrational partition function  $Q_v$  in the harmonic oscillator approximation is

$$Q_v = \frac{1}{1 - e^{-1.4388\nu/T}} \quad (5)$$

Table 3. Assignment of quantum numbers to eigenvalues for given  $J$ .

| State                   | $^2\Pi_{3/2}$ | $^2\Pi_{1/2}$ | $^2\Sigma_{1/2}$ |          |
|-------------------------|---------------|---------------|------------------|----------|
| $F$                     | 1             | 2             | 1                | 2        |
| $N$                     | $J-1/2$       | $J+1/2$       | $J-1/2$          | $J+1/2$  |
| Parity: Eigenvalue from |               |               |                  |          |
| Symmetric block         | $(-1)^{N+1}$  | $(-1)^N$      | —                | $(-1)^N$ |
| Antisymmetric block     | $(-1)^N$      | $(-1)^{N+1}$  | $(-1)^N$         | —        |

<sup>†</sup>We thank J. T. Hougen for pointing out that our notation  $s = \text{symmetric} = +$  is equivalent to the  $f$  levels and  $a = \text{antisymmetric} = -$  is equivalent to the  $e$  levels of J. M. Brown, J. T. Hougen, K.-P. Huber, J. W. C. Johns, I. Kopp, H. Lefebvre-Brion, A. J. Morer, D. A. Ramsay, J. Rostas, and R. N. Zare, *J. Molec. Spectrosc.* **58**, 500 (1975).

and  $\omega_v$  is the vibrational harmonic oscillator frequency in  $\text{cm}^{-1}$ . Huber and Herzberg<sup>7</sup> give  $\omega_v = 3737.76 \text{ cm}^{-1}$ . A comparison of the values of  $Q_v$  calculated by Eq. (5) and by direct summation of  $e^{-E_v/T}$  shows a difference of less than 0.2% at 4600°K. The rotational partition function  $Q_R$  is calculated from the actual energy levels as follows:

$$Q_R = \sum_{N'} (2J' + 1) e^{-1.4388 J'(J'+1)/T} \quad (6)$$

Chidsey and Crosley<sup>3</sup> give the Einstein A coefficient as

$$A_{v',J'}^{v'',J''} = \frac{64\pi^4}{3h} p_{v',J'}^{v'',J''} S_{J',J''} \nu^3 / (2J' + 1) \text{ sec}^{-1}, \quad (7)$$

where  $p_{v',J'}^{v'',J''}$  is the rovibrational transition probability and  $S_{J',J''}$  is the rotational line strength. Chidsey and Crosley tabulate relative values of  $A_{v',J'}^{v'',J''}$  through  $N' = 32$  for the  $A^2\Sigma - X^2\Pi(0, 0)$  band in their Table 4. They state that they calculated the line strengths  $S_{J',J''}$  based on Earls' formulas<sup>8</sup> with a  $J$ -dependent spin-orbit coupling parameter  $A$  and the rotational constants of Dieke and Crosswhite.<sup>1</sup> We have found that the use of Earls' formulas can lead to significant errors at high  $J$  in the satellite bands. (This problem is further discussed in the following section.) Therefore, we have calculated  $S_{J',J''}$  by following the method described by Hougen.<sup>4</sup> Chidsey and Crosley<sup>3</sup> have kindly provided a table of relative values for  $p_{v',J'}^{v'',J''}$  through  $J = 35.5$  prior to publication.

The  $A_{v',J'}^{v'',J''}$  may be put on an absolute basis by noting that the lifetime of a state is

$$\tau_{v',J'} = \left( \sum_{v'',J''} A_{v',J'}^{v'',J''} \right)^{-1} \text{ sec.} \quad (8)$$

Because Chidsey and Crosley<sup>3</sup> give  $A_0^0/A_0^0 \approx 0.0040$  (here the notation is  $A_{v',J'}^{v'',J''}$ ), we assume that for the  $v' = 0$  vibrational state all vibrational states other than  $v'' = 0$  make negligible contributions to  $\tau_{v',J'}$ . The best available lifetime for the rotationless ( $N' = 0$ )  $v' = 0$  state is probably that measured by German,<sup>10</sup>  $\tau_{0,1,2} = (0.688 \pm 0.007) \times 10^{-6}$  sec. There are three transitions from the  $v'' = 0$  state to the rotationless  $v' = 0$  state, namely,  ${}^P P_{1,1}(1,5)$ ,  ${}^O P_{1,2}(1,5)$ , and  ${}^R Q_{1,2}(0,5)$ . We calculate relative  $A_{v',J'}^{v'',J''}$  for all  $J'$  and  $J''$  of interest by ignoring all constant factors in Eq. (7) and normalize these by using Eq. (8).

We form the  $S_{J',J''}$  by following the method given by Hougen.<sup>4</sup> In addition to the selection rules  $\Delta J = 0, \pm 1$  and  $+\leftrightarrow -$  parity, electric dipole selection rules on  $\Omega$  give nonzero matrix elements only for  $\langle \Omega \pm 1 | \mu_x \pm i\mu_y | \Omega \rangle$  for  $\Delta\Omega = \pm 1$  and  $\langle \Omega | \mu_x | \Omega \rangle$  for  $\Delta\Omega = 0$ , where  $\mu_x, \mu_y$ , and  $\mu_z$  are electric dipole moment components in the molecule fixed axis system. In the laboratory fixed coordinate system

$$\mu_z = \frac{1}{2}(\alpha_{z_x} - i\alpha_{z_y})(\mu_x + i\mu_y) + \frac{1}{2}(\alpha_{z_x} + i\alpha_{z_y})(\mu_x - i\mu_y) + \alpha_z \mu_z, \quad (9)$$

where  $\alpha_{z_x}$ ,  $\alpha_{z_y}$ , and  $\alpha_z$  are the direction cosines between the molecule-fixed and laboratory-

Table 4. Nonzero rotational direction cosine matrix elements in  $(J'\Omega'|\mu_z|J\Omega)$  (Hund's case (a)).

|  | $J' = J+1$  | $J' = J$  | $J' = J-1$  |
|--|---|---|---|
| $\langle J \Omega \mu_z J,\Omega\rangle$   | $\left[ \frac{(J+\Omega+1)(J-\Omega+1)}{2(J+1)} \right]^{1/2}$  | $-\Omega \left[ \frac{2J+1}{2J(J+1)} \right]^{1/2}$                 | $\left[ \frac{(J+\Omega)(J-\Omega)}{2J} \right]^{1/2}$    |
| $\langle J \Omega+1 \mu_z J,\Omega\rangle$ | $-\left[ \frac{(J+\Omega+1)(J+\Omega+2)}{2(J+1)} \right]^{1/2}$ | $\left[ \frac{(J-\Omega)(J+\Omega+1)(2J+1)}{2J(J+1)} \right]^{1/2}$ | $\left[ \frac{(J-\Omega)(J-\Omega-1)}{2J} \right]^{1/2}$  |
| $\langle J \Omega-1 \mu_z J,\Omega\rangle$ | $\left[ \frac{(J-\Omega+1)(J-\Omega+2)}{2(J+1)} \right]^{1/2}$  | $\left[ \frac{(J+\Omega)(J-\Omega+1)(2J+1)}{2J(J+1)} \right]^{1/2}$ | $-\left[ \frac{(J+\Omega)(J+\Omega-1)}{2J} \right]^{1/2}$ |

Note: The phases employed here are the same as those used in Refs. 2, 4, and 11.

fixed coordinates systems. The direction cosine matrix elements are given in Table 4. The  $\mu_x$ ,  $\mu_y$ , and  $\mu_z$  are taken to be experimentally determined parameters. For lack of better information, we take  $\sqrt{(1/2)|\mu_x + i\mu_y|} = \sqrt{(1/2)|\mu_x - i\mu_y|} = \mu_x = 1$ .

Because we assume that the electronic and rotational parts of the wavefunction are separable, the electric dipole matrix elements may be written as

$$\begin{aligned} \langle \Lambda'S'\Sigma'; J'\Omega' | \mu_z | \Lambda S \Sigma; J \Omega \rangle &= \frac{1}{2} \langle \Lambda'S'\Sigma' | \mu_x + i\mu_y | \Lambda S \Sigma \rangle \langle J'\Omega' | a_{2x} - ia_{2y} | J \Omega \rangle \\ &+ \frac{1}{2} \langle \Lambda'S'\Sigma' | \mu_x - i\mu_y | \Lambda S \Sigma \rangle \langle J'\Omega' | a_{2x} + ia_{2y} | J \Omega \rangle + \langle \Lambda'S'\Sigma' | \mu_z | \Lambda S \Sigma \rangle \langle J'\Omega' | a_{2z} | J \Omega \rangle, \end{aligned} \quad (10)$$

where " has been dropped on the lower state quantities. Only one of the three terms on the r.h.s. of Eq. (10) is nonzero for any allowed transition matrix element. The electric dipole transition matrix is formed in the same basis as was the Hamiltonian matrix, that is, the Hund's case (a) basis. Selection rules in this basis are  $\Delta S = 0$ ,  $\Delta \Sigma = 0$ ,  $\Delta \Lambda = 0, \pm 1$ , and  $\Delta J = 0, \pm 1$ . Because  $\Delta \Sigma = 0$  and  $\Omega = \Lambda + \Sigma$ , the selection rule  $\Delta \Omega = \Delta \Lambda$  is obtained.

For  $^2\Sigma-^2\Pi$  transitions the last term in Eq. (10) is always zero. Because we are interested in  $^2\Sigma-^2\Pi$  transitions, we set all matrix elements of the type  $\langle ^2\Sigma | \mu_z | ^2\Sigma \rangle$  and  $\langle ^2\Pi | \mu_z | ^2\Pi \rangle$  equal to zero. This approximation is valid because these matrix elements are much smaller in magnitude than the  $\langle ^2\Sigma | \mu_z | ^2\Pi \rangle$  matrix elements and because they enter into the line strength only through weak mixing between the  $^2\Pi$  and  $^2\Sigma$  wavefunctions. The relative phases of the matrix elements are determined by following the prescription of Hougen<sup>4</sup> and Whiting and Nicholls.<sup>11</sup> Following the suggestions of Whiting and Nicholls, we have normalized the line strengths so that

$$\sum_{J'} S_{J'J''} = 2(2S+1)(2J''+1) = 4(2J''+1). \quad (11)$$

Table 4 reflects this choice of normalization.

The line strength  $S_{J'J''}$  is formed in intermediate coupling by taking  $|\langle u | \mu_z | l \rangle|^2$ , where  $|u\rangle$  represents the eigenvector of the  $^2\Sigma$  state,  $|l\rangle$  represents the eigenvector of the  $^2\Pi$  state, and  $\mu_z$  now represents the  $6 \times 6$  transition matrix. However, the eigenvectors formed during diagonalization of the energy matrices are in the Kronig transformed basis; therefore, the dipole matrix must also be transformed into this basis. Using the Kronig transformed wavefunctions given by Eq. (1), the Kronig transformed dipole matrix elements have the form

$$\begin{aligned} \langle J'\Omega'\delta' | \mu_z | J\Omega\delta \rangle &= \frac{1}{2} (\langle J'\Omega' | \mu_z | J\Omega\delta \rangle + \delta \langle J'\Omega' | \mu_z | J-\Omega \rangle) \\ &+ \delta' \langle J'-\Omega' | \mu_z | J\Omega \rangle + \delta\delta' \langle J'-\Omega' | \mu_z | J-\Omega \rangle \end{aligned} \quad (12)$$

and, if we let  $\mu_z^\xi$  be the matrix of the  $\langle J'\Omega'\delta' | \mu_z | J\Omega\delta \rangle$ ,

$$S_{J'J''} = |\langle J'\Omega'\delta' | \mu_z^\xi | J\Omega\delta \rangle|^2. \quad (13)$$

To our knowledge, the  $^2\Sigma-^2\Pi$  transition matrices have not been published elsewhere. We show them for the P, Q, and R branches in Tables 5-7. The twelve branches correspond to the four  $3 \times 3$  blocks in the Kronig basis as follows:

$$\left( \begin{array}{c|c} \begin{array}{c} a \leftarrow a \\ {}^P P_{11}, {}^R R_{11}, {}^O P_{12}, {}^O R_{12} \end{array} & \begin{array}{c} a \leftarrow s \\ {}^O Q_{11}, {}^P Q_{12} \end{array} \\ \hline \begin{array}{c} s \leftarrow a \\ {}^O Q_{22}, {}^R Q_{21} \end{array} & \begin{array}{c} s \leftarrow s \\ {}^P P_{22}, {}^R R_{22}, {}^O P_{21}, {}^S R_{21} \end{array} \end{array} \right) \quad (14)$$

For the Q-branch lines, the only nonzero  $3 \times 3$  blocks are those for  $a \leftarrow s$  and  $s \leftarrow a$ , while, for the R- and P-branch lines, the only nonzero  $3 \times 3$  blocks are those for  $a \leftarrow a$  and  $s \leftarrow s$ . When forming line strengths, the appropriate block must be substituted into Eq. (13) for  $\mu_z^\xi$ . For





Table 6. Q-branch  $^2\Sigma - ^2\Pi$  transition matrix.

| 1) Hund's case (a) basis |                    |                    |                   | 2) Kronig basis |                 |                |                |                |                |
|--------------------------|--------------------|--------------------|-------------------|-----------------|-----------------|----------------|----------------|----------------|----------------|
|                          | $2^2\Sigma_{-1/2}$ | $2^2\Sigma_{-1/2}$ | $2^2\Sigma_{1/2}$ | $2^2\Pi_{-1/2}$ | $2^2\Pi_{-1/2}$ | $2^2\Pi_{1/2}$ | $2^2\Pi_{1/2}$ | $2^2\Pi_{3/2}$ | $2^2\Pi_{3/2}$ |
| $2^2\Sigma_{3/2}$        | 0                  | 0                  | -c                | 0               | 0               | 0              | 0              | 0              | 0              |
| $2^2\Sigma_{1/2}$        | 0                  | 0                  | 0                 | -v              | 0               | 0              | 0              | 0              | 0              |
| $2^2\Sigma_{-1/2}$       | -c                 | 0                  | 0                 | 0               | v               | 0              | 0              | 0              | 0              |
| $2^2\Pi_{3/2}$           | 0                  | -v                 | 0                 | 0               | 0               | 0              | c              | 0              | 0              |
| $2^2\Pi_{1/2}$           | 0                  | 0                  | v                 | 0               | 0               | 0              | 0              | 0              | 0              |
| $2^2\Pi_{-1/2}$          | 0                  | 0                  | 0                 | 0               | 0               | 0              | 0              | 0              | 0              |

$$c = \frac{(J-1/2)(J+3/2)(2J+1)}{2J(J+1)}^{1/2} v_2$$

$$v = \frac{(J+1/2)(2J+1)}{2J(J+1)}^{1/2} v_2$$

where  $v_2 = \sqrt{6} |v_{2,1} v_{2,2}| - 1$



example, to generate the  $Q_1$  line strength we form

$$S^Q = |\langle \psi_{n_1,2}^s | (a \leftarrow s) | \psi_{n_1,2}^t \rangle|^2 \quad (15)$$

### 3. RESULTS AND DISCUSSION

Line strengths, Einstein A coefficients, intensities, and transition frequencies have been calculated for all branches of the  $A^2\Sigma-X^2\Pi(0,0)$  OH spectrum through  $J = 15.5$  at  $240^\circ\text{K}$  for atmospheric applications and through  $J = 40.5$  at  $4600^\circ\text{K}$  for high temperature applications. These calculated values are shown in Tables 8 and 9, respectively. The total band intensities (by summation of the individual lines) are  $2.7948 \times 10^4 \text{ cm}^{-1}/\text{atm-cm}$  at  $240^\circ\text{K}$  and  $8.6863 \times 10^2 \text{ cm}^{-1}/\text{atm-cm}$  at  $4600^\circ\text{K}$ . Line intensities are plotted at these two temperatures in Fig. 1. Some caution must be exercised in using high  $J$  data from Table 9. The spectroscopic constants<sup>2</sup> used here were determined from data<sup>2</sup> which included transitions through  $J = 25.5$ . Although these constants allow prediction of that data to within  $0.1 \text{ cm}^{-1}$  maximum error and a standard deviation of  $\sim 0.03 \text{ cm}^{-1}$  (the hyperfine structure is neglected here), such accuracy cannot be expected for all lines between  $J = 25.5$  and  $40.5$ . Uncertainties in the calculation of energy levels at these high  $J$  cause proportionally smaller uncertainties in the energy eigenvectors (wavefunctions) and in quantities calculated using the eigenvectors (line strengths, Einstein A coefficients, and intensities).

Chidsey and Crosley<sup>9</sup> list  $p_{v'J'}$  through  $J = 35.5$ . We have extrapolated  $p_{v'J'}$  for  $J = 36.5$ – $40.5$ . Although the dependence of  $p_{v'J'}$  on  $J$  is quite linear for P, Q, and R transition probabilities between  $J = 25.5$  and  $35.5$ , extrapolated  $p_{v'J'}$  used to calculate Einstein A coefficients and intensities at higher  $J$  must be used with caution.

Although we list four digits for Einstein A coefficients and intensities in Tables 8 and 9, the absolute uncertainties of these quantities cannot be less than 1%, because German's<sup>10</sup>  $\tau_{0,1,2}$  has a 1% quoted uncertainty and because Chidsey and Crosley's<sup>9</sup>  $p_{v'J'}$  are quoted to three significant digits. The relative uncertainties are limited by the relative accuracy of the  $p_{v'J'}$  and the line strengths. These relative uncertainties should be less than 0.5% for  $J$  less than 25.5 and are probably less than 1% for  $J$  less than 35.5.

Our calculated line strengths have been checked for accuracy by comparison with values calculated using Earls<sup>11</sup> algebraic formulas (these formulas are equivalent to those of Kovacs<sup>12</sup> for  $^2\Sigma-^2\Pi$  transitions). When centrifugal and higher order distortion and  $\Sigma-\Pi$  interactions are

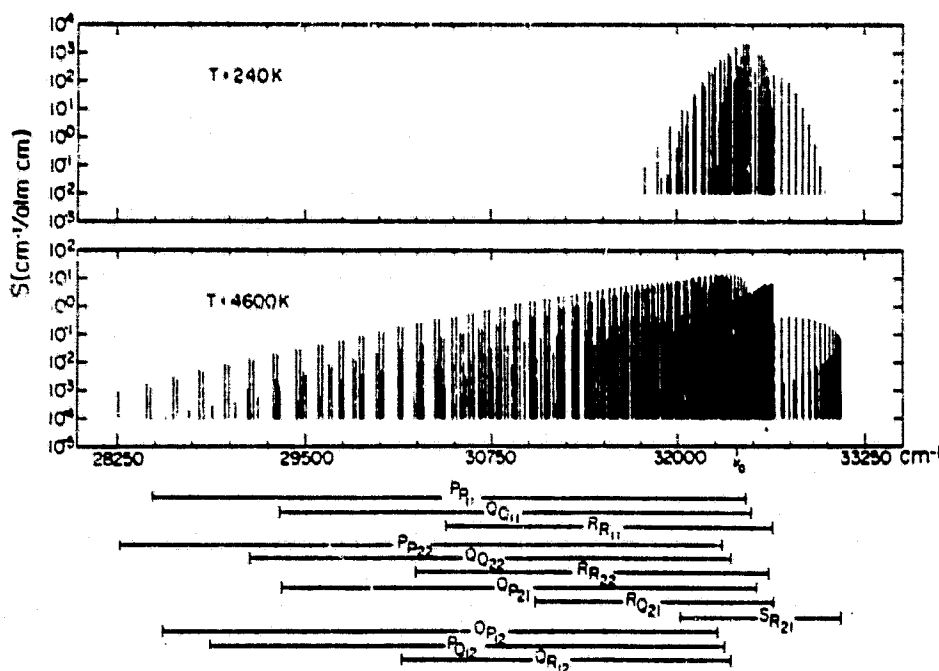


Fig. 1. Line intensities and positions for the  $A^2\Sigma-X^2\Pi(0,0)$  band of OH. Only lines with intensity greater than  $10^{-5}$  the intensity of the strongest line have been plotted.

Table 8. Line parameters for the  $A^1\Sigma^+ - X^1\Pi(0,0)$  OH band at 240°K.

| J'   | J''  | Lower energy<br>vacuum cm <sup>-1</sup> | Transition      | Frequency<br>vacuum cm <sup>-1</sup> | Wavelength<br>SIP angstroms | Intensity<br>cm <sup>-2</sup> atm <sup>-1</sup> | Intensity<br>cm/molecule | Einstein<br>sec <sup>-1</sup> | A Line<br>strength | Number |
|------|------|---|-----------------|--------------------------------------|-----------------------------|---|--------------------------|-------------------------------|--------------------|--------|
| 14.5 | 15.5 | 4939.922                                | 0 P 1 2(15.5)   | 3075.003                             | 3227.4696                   | 2.110E-11                                       | 6.925E-31                | 3.910E+03                     | 2.20361E-01        | 1      |
| 13.5 | 14.5 | 4377.419                                | 0 P 1 2(14.5)   | 3104.603                             | 3216.0096                   | 6.649E-10                                       | 2.174E-29                | 4.547E+03                     | 2.31060E-01        | 2      |
| 12.5 | 13.5 | 3846.059                                | 0 P 1 2(13.5)   | 3131.092                             | 3205.0351                   | 1.729E-08                                       | 5.659E-20                | 5.329E+03                     | 2.32803E-01        | 3      |
| 11.5 | 12.5 | 3348.000                                | 0 P 1 2(12.5)   | 3126.666                             | 3194.3051                   | 3.704E-07                                       | 1.213E-26                | 6.208E+03                     | 2.36976E-01        | 4      |
| 10.5 | 11.5 | 2804.110                                | 0 P 1 2(11.5)   | 3150.949                             | 3183.0992                   | 6.515E-06                                       | 2.133E-25                | 7.408E+03                     | 2.72606E-01        | 5      |
| 14.5 | 15.5 | 4932.933                                | 0 P 2 2(15.5)   | 3146.396                             | 3177.6003                   | 1.623E-09                                       | 5.307E-29                | 2.965E+05                     | 1.59636E+01        | 6      |
| 15.5 | 15.5 | 4932.933                                | 0 P 0 1 2(15.5) | 3146.396                             | 3177.6003                   | 7.679E-11                                       | 2.444E-30                | 1.204E+04                     | 7.57344E-01        | 7      |
| 9.5  | 10.5 | 2453.149                                | 0 P 1 2(10.5)   | 3190.667                             | 3173.4193                   | 9.371E-05                                       | 3.064E-24                | 9.003E+03                     | 2.90335E-01        | 8      |
| 13.5 | 14.5 | 4371.365                                | 0 P 2 2(14.5)   | 3154.660                             | 3169.6197                   | 4.517E-08                                       | 1.477E-27                | 3.067E+05                     | 1.49196E+01        | 9      |
| 14.5 | 14.5 | 4371.365                                | 0 P 0 1 2(14.5) | 3154.660                             | 3169.6197                   | 2.333E-09                                       | 7.428E-29                | 1.476E+04                     | 7.91566E-01        | 10     |
| 14.5 | 15.5 | 4341.046                                | 0 P 1 1(15.5)   | 31573.139                            | 3166.3329                   | 5.750E-08                                       | 1.800E-27                | 3.059E+05                     | 1.623750E+01       | 11     |
| 8.5  | 9.5  | 2056.568                                | 0 P 1 2(9.5)    | 31595.731                            | 3165.0607                   | 1.059E-03                                       | 3.595E-23                | 3.595E+04                     | 1.80366E-01        | 12     |
| 12.5 | 13.5 | 3841.676                                | 0 P 2 2(13.5)   | 31617.646                            | 3161.5977                   | 1.033E-06                                       | 3.170E-26                | 3.170E+05                     | 1.30917E+01        | 13     |
| 13.5 | 13.5 | 3841.676                                | 0 P 0 1 2(13.5) | 31623.625                            | 3161.5977                   | 6.019E-08                                       | 1.960E-27                | 1.710E+04                     | 0.30293E-01        | 14     |
| 13.5 | 14.5 | 3818.759                                | 0 P 1 1(14.5)   | 31651.363                            | 3158.5092                   | 1.337E-06                                       | 4.371E-26                | 3.172E+05                     | 1.52695E+01        | 15     |
| 7.5  | 8.5  | 1694.914                                | 0 P 1 2(8.5)    | 3155.980                             | 3154.6534                   | 1.040E-12                                       | 3.420E-32                | 1.352E+04                     | 3.32902E-01        | 16     |
| 11.5 | 12.5 | 3344.522                                | 0 P 2 2(12.5)   | 31691.411                            | 3154.5157                   | 1.926E-05                                       | 6.293E-25                | 3.267E+05                     | 1.28593E+01        | 17     |
| 12.5 | 12.5 | 3344.522                                | 0 P 0 1 2(12.5) | 31694.220                            | 3154.5157                   | 2.200E-06                                       | 4.307E-26                | 2.805E+04                     | 0.74207E-01        | 18     |
| 12.5 | 13.5 | 3311.902                                | 0 P 1 1(13.5)   | 31726.749                            | 3151.8001                   | 2.547E-05                                       | 8.330E-25                | 3.209E+05                     | 1.42615E+01        | 19     |
| 10.5 | 11.5 | 2808.525                                | 0 P 2 2(11.5)   | 31762.632                            | 3167.4639                   | 2.920E-04                                       | 9.549E-24                | 3.363E+05                     | 1.40217E+01        | 20     |
| 11.5 | 11.5 | 2808.525                                | 0 P 0 1 2(11.5) | 31765.021                            | 3167.2054                   | 2.235E-05                                       | 7.310E-25                | 2.359E+04                     | 9.29697E-01        | 21     |
| 6.5  | 7.5  | 1360.720                                | 0 P 1 2(7.5)    | 31701.413                            | 3145.5021                   | 0.077E-02                                       | 2.641E-21                | 1.695E+04                     | 3.57791E-01        | 22     |
| 11.5 | 12.5 | 2846.009                                | 0 P 1 1(12.5)   | 31799.656                            | 3163.7472                   | 3.954E-04                                       | 1.293E-23                | 3.402E+05                     | 1.32510E+01        | 23     |
| 9.5  | 10.5 | 2450.279                                | 0 P 2 2(10.5)   | 31830.303                            | 3146.7625                   | 3.574E-03                                       | 1.170E-22                | 3.449E+05                     | 1.07700E+01        | 24     |
| 10.5 | 10.5 | 2450.279                                | 0 P 0 1 2(10.5) | 31832.700                            | 3146.5061                   | 3.195E-04                                       | 1.045E-23                | 2.801E+04                     | 0.80064E-01        | 25     |
| 10.5 | 11.5 | 2413.613                                | 0 P 1 1(11.5)   | 31869.446                            | 3136.0927                   | 4.904E-02                                       | 1.530E-22                | 3.510E+05                     | 1.22482E+01        | 26     |
| 5.5  | 6.5  | 1070.509                                | 0 P 1 2(6.5)    | 31869.705                            | 3136.0672                   | 5.003E-01                                       | 1.453E-20                | 2.162E+04                     | 3.04410E-01        | 27     |
| 8.5  | 9.5  | 2054.353                                | 0 P 2 2(9.5)    | 31895.203                            | 3136.3516                   | 3.525E-02                                       | 1.153E-21                | 3.532E+05                     | 0.72727E+00        | 28     |
| 9.5  | 9.5  | 2054.353                                | 0 P 0 1 2(9.5)  | 31897.663                            | 3136.1373                   | 3.724E-03                                       | 1.221E-22                | 3.359E+04                     | 1.04530E+00        | 29     |
| 9.5  | 10.5 | 2015.036                                | 0 P 1 1(10.5)   | 31936.701                            | 3136.1373                   | 5.079E-02                                       | 1.661E-21                | 3.290E+05                     | 1.12265E+01        | 30     |
| 4.5  | 5.5  | 824.013                                 | 0 P 1 2(5.5)    | 31954.665                            | 3128.5267                   | 2.476E-08                                       | 8.092E-28                | 2.819E+04                     | 4.10930E-01        | 31     |
| 7.5  | 8.5  | 1693.290                                | 0 P 2 2(8.5)    | 31957.040                            | 3128.2934                   | 2.779E-01                                       | 9.009E-21                | 3.611E+05                     | 6.66026E+00        | 32     |
| 8.5  | 8.5  | 1693.290                                | 0 P 0 1 2(8.5)  | 31959.000                            | 3128.1015                   | 3.530E-02                                       | 1.154E-21                | 4.077E+04                     | 1.11859E+00        | 33     |
| 15.5 | 15.5 | 4939.902                                | 0 P 2 2(15.5)   | 31963.173                            | 3127.6939                   | 3.010E-09                                       | 9.442E-29                | 5.549E+05                     | 3.12030E+01        | 34     |
| 8.5  | 9.5  | 1650.790                                | 0 P 1 1(9.5)    | 32001.569                            | 3123.9478                   | 4.172E-01                                       | 1.364E-20                | 3.745E+05                     | 1.02106E+01        | 35     |
| 6.5  | 7.5  | 1367.617                                | 0 P 2 2(7.5)    | 32015.507                            | 3122.5733                   | 1.740E+00                                       | 5.609E-20                | 3.408E+05                     | 7.59004E+00        | 36     |
| 14.5 | 14.5 | 4377.619                                | 0 P 0 2 2(14.5) | 32015.910                            | 3122.5417                   | 4.436E-08                                       | 2.959E-27                | 2.819E+04                     | 2.92491E+01        | 37     |
| 7.5  | 7.5  | 1367.619                                | 0 P 0 1 2(7.5)  | 32017.324                            | 3122.4330                   | 2.712E-01                                       | 0.076E-21                | 5.020E+04                     | 1.20092E+00        | 38     |
| 15.5 | 14.5 | 4377.619                                | 0 P 1 2(14.5)   | 32019.325                            | 3122.2007                   | 1.634E-09                                       | 4.690E-25                | 9.105E+03                     | 5.12512E-01        | 39     |
| 3.5  | 4.5  | 600.194                                 | 0 P 1 2(4.5)    | 32035.976                            | 3120.5450                   | 9.005E-08                                       | 3.154E-19                | 3.056E+04                     | 4.32924E-01        | 40     |
| 14.5 | 15.5 | 4351.310                                | 0 P 2 1(15.5)   | 32042.010                            | 3119.9973                   | 1.000E-09                                       | 1.000E-29                | 1.000E+00                     | 5.57413E-01        | 41     |
| 15.5 | 15.5 | 4351.310                                | 0 P 0 1 1(15.5) | 32045.433                            | 3119.6649                   | 1.026E-07                                       | 3.354E-27                | 5.577E+05                     | 3.12011E+01        | 42     |
| 7.5  | 8.5  | 1321.252                                | 0 P 1 1(8.5)    | 32063.698                            | 3117.8005                   | 2.751E-08                                       | 0.997E-28                | 3.060E+05                     | 9.19253E+00        | 43     |
| 13.5 | 13.5 | 3846.059                                | 0 P 2 2(13.5)   | 32064.966                            | 3117.7702                   | 1.939E-06                                       | 6.391E-26                | 5.064E+05                     | 2.72106E+01        | 44     |
| 14.5 | 13.5 | 3846.059                                | 0 P 1 2(13.5)   | 32068.126                            | 3117.4571                   | 3.742E-08                                       | 1.224E-27                | 1.856E+04                     | 5.40150E-01        | 45     |
| 5.5  | 6.5  | 1077.054                                | 0 P 2 2(6.5)    | 32078.760                            | 3117.2004                   | 0.575E+00                                       | 2.004E-19                | 3.737E+05                     | 6.52103E+00        | 46     |
| 6.5  | 6.5  | 1077.054                                | 0 P 0 1 2(6.5)  | 32072.279                            | 3117.0534                   | 1.600E+00                                       | 5.493E-20                | 6.270E+04                     | 1.29194E+00        | 47     |

|      |      |          |   |   |   |              |           |           |           |           |           |              |     |
|------|------|----------|---|---|---|--------------|-----------|-----------|-----------|-----------|-----------|--------------|-----|
| 13.5 | 14.5 | 3019.156 | - | 0 | 2 | 1 1 1 4 .5 1 | 32092.600 | 3115.0709 | 4.939E-00 | 1.615E-27 | 1.267E+06 | 5.05109E-01  | 68  |
| 14.5 | 14.5 | 3019.156 | - | 0 | 0 | 1 1 1 4 .5 1 | 32095.029 | 3115.7663 | 2.396E-06 | 7.035E-26 | 5.739E+05 | 2.91665E+01  | 69  |
| 12.5 | 12.5 | 3168.000 | 0 | 0 | 2 | 2 1 2 .5 1   | 32110.200 | 3113.3722 | 3.630E-05 | 1.190E-24 | 6.082E+05 | 2.91666E+01  | 50  |
| 2.5  | 2.5  | 429.275  | - | 0 | 1 | 1 2 1 3 .5 1 | 32113.223 | 3113.0001 | 2.091E+01 | 9.659E-19 | 5.179E+04 | 4.09599E-01  | 51  |
| 13.5 | 12.5 | 3368.000 | 0 | 0 | R | 1 2 1 2 .5 1 | 32113.222 | 3113.0792 | 0.042E-07 | 2.630E-26 | 1.237E+06 | 5.71279E-01  | 52  |
| 4.5  | 5.5  | 426.525  | 0 | P | 2 | 2 1 9 .5 1   | 32122.605 | 3112.1992 | 3.293E+01 | 3.077E-13 | 3.785E+05 | 5.63172E+00  | 53  |
| 6.5  | 7.5  | 1026.730 | - | P | P | 1 1 1 7 .5 1 | 32123.403 | 3112.0925 | 1.669E+01 | 4.730E-19 | 6.907E+05 | 0.17260E+00  | 54  |
| 5.5  | 5.5  | 024.525  | 0 | 0 | 0 | 1 2 1 5 .5 1 | 32123.609 | 3112.0664 | 0.346E+00 | 2.729E-19 | 7.991E+04 | 1.30079E+00  | 55  |
| 12.5 | 13.5 | 3319.355 | 0 | 0 | P | 2 1 1 3 .5 1 | 32139.725 | 3110.5120 | 1.060E-05 | 3.699E-26 | 1.679E+06 | 6.16716E+01  | 56  |
| 13.5 | 12.5 | 3319.355 | 0 | 0 | 0 | 1 1 1 3 .5 1 | 32142.747 | 3110.2196 | 4.570E-05 | 1.697E-24 | 5.000E+05 | 2.71260E+01  | 47  |
| 11.5 | 11.5 | 2006.110 | - | 0 | 0 | 2 1 1 1 .5 1 | 32151.022 | 3109.3416 | 5.539E-04 | 1.011E-23 | 6.120E+05 | 2.31170E+01  | 58  |
| 12.5 | 11.5 | 2006.110 | - | 0 | R | 1 2 1 1 .5 1 | 32154.640 | 3119.0691 | 1.649E-05 | 4.641E-25 | 1.449E+06 | 6.06610E+01  | 59  |
| 3.5  | 4.5  | 600.100  | - | P | P | 2 2 1 4 .5 1 | 32170.237 | 3107.5617 | 9.696E+01 | 3.071E-10 | 3.039E+05 | 4.33999E+00  | 60  |
| 4.5  | 4.5  | 600.104  | - | P | 0 | 1 2 1 4 .5 1 | 32171.290 | 3107.4600 | 3.292E+01 | 1.077E-10 | 1.037E+05 | 1.64361E+00  | 61  |
| 5.5  | 6.5  | 767.650  | 0 | P | 0 | 1 2 1 6 .5 1 | 32180.756 | 3106.5659 | 6.067E+01 | 1.906E-10 | 4.161E+05 | 7.15200E+00  | 62  |
| 11.5 | 12.5 | 2052.605 | - | 0 | P | 2 1 1 2 .5 1 | 32183.440 | 3106.2060 | 1.095E-05 | 6.202E-25 | 1.737E+06 | 6.32643E-01  | 63  |
| 1.5  | 2.5  | 200.769  | 0 | 0 | P | 1 2 1 2 .5 1 | 32185.009 | 3106.6592 | 6.333E+01 | 2.071E-10 | 7.357E+05 | 0.133556E-01 | 64  |
| 12.5 | 12.5 | 2052.605 | - | 0 | 0 | 1 1 1 2 .5 1 | 32186.266 | 3106.0161 | 7.126E-04 | 2.330E-23 | 6.029E+05 | 2.50914E+01  | 65  |
| 16.5 | 10.5 | 2633.169 | 0 | 0 | 0 | 2 2 1 0 .5 1 | 32189.707 | 3105.6743 | 5.019E-03 | 2.230E-22 | 6.229E+05 | 2.10604E+01  | 66  |
| 11.5 | 10.5 | 2433.169 | 0 | 0 | R | 1 2 1 0 .5 1 | 32192.397 | 3135.4225 | 2.046E+04 | 6.692E-24 | 1.711E+06 | 6.46105E-01  | 67  |
| 2.5  | 3.5  | 429.650  | 0 | P | P | 2 1 1 3 .5 1 | 32213.092 | 3103.3503 | 2.127E+02 | 3.079E-10 | 3.039E+05 | 3.23670E+00  | 68  |
| 3.5  | 3.5  | 429.650  | 0 | P | 0 | 1 2 1 3 .5 1 | 32214.713 | 3103.2712 | 1.014E+02 | 3.370E-10 | 1.377E+05 | 1.55030E+00  | 69  |
| 10.5 | 11.5 | 2419.001 | 0 | 0 | P | 2 1 1 1 .5 1 | 32223.055 | 3132.3960 | 2.766E-04 | 9.040E-24 | 2.060E+06 | 6.91759E-01  | 70  |
| 9.5  | 9.5  | 2056.560 | - | 0 | 0 | 2 2 1 9 .5 1 | 32224.000 | 3102.2122 | 5.746E-02 | 2.206E-21 | 6.296E+05 | 1.09962E+01  | 71  |
| 11.5 | 11.5 | 2419.001 | 0 | 0 | 0 | 1 1 1 1 .5 1 | 32226.666 | 3102.1396 | 0.906E-03 | 2.939E-22 | 6.139E+05 | 2.30299E+01  | 72  |
| 10.5 | 9.5  | 2056.560 | - | P | P | 1 1 1 5 .5 1 | 32226.923 | 3102.1369 | 2.611E+02 | 7.060E-23 | 2.011E+06 | 6.90930E-01  | 73  |
| 4.5  | 5.5  | 543.575  | - | P | P | 1 1 2 1 .5 1 | 32235.923 | 3101.2312 | 2.611E+02 | 6.576E-10 | 4.319E+05 | 6.13324E+00  | 74  |
| 1.5  | 2.5  | 209.041  | - | P | P | 2 2 1 2 .5 1 | 32252.060 | 3099.6007 | 3.293E+02 | 1.077E-17 | 3.040E+05 | 2.19001E+00  | 75  |
| 5    | 1.5  | 107.691  | - | 0 | 0 | 1 2 1 5 .5 1 | 32253.049 | 3099.5025 | 0.761E+01 | 2.065E-10 | 1.114E+05 | 3.10162E-01  | 76  |
| 2.5  | 2.5  | 209.361  | - | 0 | 0 | 1 2 1 2 .5 1 | 32253.667 | 3099.5463 | 2.640E+02 | 7.070E-10 | 1.079E+05 | 1.57235E+00  | 77  |
| 0.5  | 0.5  | 1696.914 | 0 | 0 | 0 | 2 2 1 0 .5 1 | 32256.722 | 3099.4217 | 5.330E-01 | 1.746E-20 | 6.349E+05 | 1.69230E+01  | 78  |
| 9.5  | 0.5  | 1696.914 | 0 | 0 | R | 1 2 1 0 .5 1 | 32256.962 | 3099.2122 | 7.9.9E-22 | 7.9.9E-22 | 2.650E+04 | 7.41015E-01  | 79  |
| 9.5  | 10.5 | 2019.633 | - | 0 | P | 2 1 1 0 .5 1 | 32261.029 | 3090.8150 | 3.295E-03 | 1.077E-22 | 2.650E+04 | 7.41015E-01  | 80  |
| 10.5 | 10.5 | 2019.633 | - | 0 | 0 | 1 1 1 0 .5 1 | 32263.626 | 3090.5056 | 9.153E-02 | 2.993E-21 | 6.236E+05 | 2.09700E+01  | 81  |
| 7.5  | 7.5  | 1360.720 | - | 0 | 0 | 2 2 1 7 .5 1 | 32281.659 | 3096.0392 | 3.359E+00 | 1.090E-19 | 6.360E+05 | 1.49631E+01  | 82  |
| 4.5  | 7.5  | 1360.720 | - | 0 | R | 1 2 1 7 .5 1 | 32283.579 | 3096.6512 | 1.776E-01 | 5.000E-21 | 2.991E+06 | 7.97604E-01  | 83  |
| 5    | 1.5  | 107.751  | 0 | P | P | 2 2 1 5 .5 1 | 32286.675 | 3096.3716 | 3.111E+02 | 1.017E-17 | 3.970E+05 | 1.10194E+00  | 84  |
| 1.5  | 1.5  | 107.751  | 0 | P | 0 | 1 2 1 5 .5 1 | 32286.027 | 3096.3196 | 6.100E+02 | 1.367E-17 | 2.667E+05 | 1.40900E+00  | 85  |
| 3.5  | 4.5  | 355.105  | 0 | P | 1 | 1 1 4 .5 1   | 32299.066 | 3096.1250 | 5.264E+02 | 1.719E-17 | 4.563E+05 | 5.12107E+00  | 86  |
| 0.5  | 9.5  | 1656.577 | 0 | 0 | P | 2 1 9 .5 1   | 32295.059 | 3095.5502 | 3.207E-02 | 1.049E-21 | 2.999E+06 | 7.05546E-01  | 87  |
| 9.5  | 9.5  | 1656.577 | 0 | 0 | 0 | 1 1 9 .5 1   | 32297.240 | 3095.3616 | 7.690E-01 | 2.649E-20 | 6.304E+05 | 1.09017E+01  | 88  |
| 6.5  | 6.5  | 1070.509 | 0 | 0 | 0 | 2 2 1 0 .5 1 | 32306.695 | 3096.6269 | 1.666E+01 | 5.641E-19 | 6.332E+05 | 1.215556E+01 | 89  |
| 7.5  | 6.5  | 1070.509 | 0 | 0 | R | 1 2 1 0 .5 1 | 32306.433 | 3096.4605 | 1.106E+00 | 3.616E-20 | 3.602E+06 | 0.59222E-01  | 90  |
| 5.5  | 5.5  | 126.669  | - | 0 | 0 | 1 2 1 .5 1   | 32314.091 | 3093.7271 | 5.635E+02 | 1.777E-17 | 6.010E+05 | 1.33333E+00  | 91  |
| 5.5  | 5.5  | 026.013  | - | 0 | 0 | 2 2 1 5 .5 1 | 32323.040 | 3092.7972 | 6.636E+01 | 2.105E-10 | 6.252E+05 | 1.00667E+01  | 92  |
| 6.5  | 5.5  | 926.013  | - | 0 | R | 1 2 1 5 .5 1 | 32325.320 | 3092.6524 | 5.512E+00 | 1.002E-19 | 4.509E+06 | 9.23700E-01  | 93  |
| 7.5  | 0.5  | 1326.291 | - | 0 | P | 2 1 0 .5 1   | 32326.047 | 3092.5020 | 2.564E-01 | 0.320E-21 | 3.702E+06 | 0.50667E-01  | 94  |
| 0.5  | 0.5  | 1326.291 | - | 0 | 0 | 1 1 0 .5 1   | 32329.067 | 3092.3952 | 4.907E+00 | 6.600E-19 | 6.367E+05 | 1.60236E+01  | 95  |
| 4.5  | 4.5  | 600.196  | 0 | 0 | 0 | 2 2 1 4 .5 1 | 32330.736 | 3091.3693 | 1.014E+02 | 6.600E-10 | 6.099E+05 | 4.50160E+00  | 96  |
| 5.5  | 4.5  | 600.196  | 0 | 0 | R | 1 2 1 4 .5 1 | 32343.020 | 3091.2466 | 2.177E+01 | 7.126E-19 | 5.779E+06 | 4.05130E-01  | 97  |
| 2.5  | 3.5  | 201.922  | - | P | P | 1 1 3 .5 1   | 32363.567 | 3091.1943 | 1.066E+03 | 3.007E-17 | 4.956E+05 | 4.13042E+00  | 98  |
| 5.5  | 5.5  | 126.291  | 0 | 0 | 0 | 2 2 1 .5 1   | 32367.936 | 3090.6902 | 5.666E+02 | 1.701E-17 | 4.026E+05 | 1.33333E+00  | 99  |
| 1.5  | 1.5  | 126.291  | 0 | 0 | R | 1 2 1 .5 1   | 32360.207 | 3090.4565 | 2.717E+02 | 0.006E-10 | 1.264E+05 | 6.66666E-01  | 100 |

Table 8 (Cont'd).

| J' J'' | Lower energy<br>vacuum cm <sup>-1</sup> | Transition     | Frequency<br>vacuum cm <sup>-1</sup> | Wavelength<br>STP angstroms | Intensity<br>cm <sup>-2</sup> -atm <sup>-1</sup> | Intensity<br>cm/molecule | Einstein<br>sec <sup>-1</sup> | A Line<br>strength | Number |
|--------|---|----------------|--------------------------------------|-----------------------------|--|--------------------------|-------------------------------|--------------------|--------|
| 3-5    | 429,275 -                               | 0 0 2 21 3-51  | 32349.150                            | 3090.3741                   | 6.209E+02  | 1.49E-17                 | 5.04E+05                      | 6.52912E+00        | 101    |
| 4-5    | 429,275 -                               | 0 0 1 21 3-51  | 32350.203                            | 3090.2735                   | 6.711E+01  | 2.19E-10                 | 7.31E+06                      | 1.02990E+00        | 102    |
| 6-5    | 1029,092 0                              | 0 0 2 11 7-51  | 32356.112                            | 3089.9001                   | 1.641E+00  | 5.36E-20                 | 4.69E+04                      | 9.31010E-01        | 103    |
| 1-5    | 107,691 -                               | 0 0 2 21 1-51  | 32356.410                            | 3089.6717                   | 7.776E+02  | 2.94E-17                 | 6.97E+05                      | 2.75253E+00        | 104    |
| 2-5    | 200,769 0                               | 0 0 2 21 2-51  | 32356.501                            | 3089.6553                   | 6.904E+02  | 2.894E-17                | 5.46E+05                      | 6.55550E+00        | 105    |
| 2-5    | 107,691 -                               | 0 0 1 21 1-51  | 32356.997                            | 3089.6156                   | 2.637E+02  | 6.62E-10                 | 1.12E+05                      | 9.37233E-01        | 106    |
| 3-5    | 200,769 0                               | 0 0 1 21 2-51  | 32355.401                            | 3089.7770                   | 1.571E+02  | 5.137E-10                | 9.221E+04                     | 1.03070E+00        | 107    |
| 7-5    | 1029,092 0                              | 0 0 1 11 7-51  | 32355.050                            | 3089.7342                   | 2.559E+01  | 0.36E-19                 | 6.357E+05                     | 1.47340E+01        | 108    |
| 5-5    | 769,216 -                               | 0 0 2 11 6-51  | 32379.405                            | 3087.4067                   | 0.504E+00  | 2.007E-19                | 5.99E+04                      | 1.01636E+00        | 109    |
| 6-5    | 769,216 -                               | 0 0 1 11 6-51  | 32380.917                            | 3087.3422                   | 1.055E+02  | 3.45E-10                 | 6.317E+05                     | 1.26352E+01        | 110    |
| 1-5    | 83,719 0                                | 0 0 1 11 2-51  | 32390.059                            | 3086.3945                   | 1.679E+03  | 5.40E-17                 | 5.77E+05                      | 3.10620E+00        | 111    |
| 4-5    | 544,009 0                               | 0 0 2 11 5-51  | 32402.122                            | 3085.3217                   | 3.642E+01  | 1.19E-10                 | 7.94E+04                      | 1.11315E+00        | 112    |
| 5-5    | 544,009 0                               | 0 0 1 11 5-51  | 32403.405                            | 3085.1995                   | 3.412E+02  | 1.11E-17                 | 6.21E+05                      | 1.05266E+01        | 113    |
| 1-5    | 126,449 -                               | 0 0 2 21 1-51  | 32415.452                            | 3084.0520                   | 2.721E+02  | 0.917E-10                | 1.21E+05                      | 6.66664E-01        | 116    |
| 3-5    | 355,900 -                               | 0 0 2 11 6-51  | 32422.526                            | 3083.3000                   | 1.250E+02  | 4.00E-10                 | 1.10E+05                      | 1.22124E+00        | 115    |
| 4-5    | 355,900 -                               | 0 0 1 11 6-51  | 32423.579                            | 3083.2790                   | 0.5-1E+02  | 2.79E-17                 | 6.02E+05                      | 0.41497E+00        | 116    |
| 5-5    | 0,000 -                                 | 0 0 1 11 5-51  | 32440.940                            | 3081.6677                   | 2.060E+03  | 6.737E-17                | 0.611E+05                     | 2.35649E+00        | 117    |
| 2-5    | 202,370 0                               | 0 0 2 11 3-51  | 32448.940                            | 3081.6259                   | 3.452E+02  | 1.12E-17                 | 1.61E+05                      | 1.33651E+00        | 118    |
| 3-5    | 202,370 0                               | 0 0 1 11 3-51  | 32441.001                            | 3081.5479                   | 1.621E+03  | 5.30E-17                 | 5.70E+05                      | 6.31440E+00        | 119    |
| 2-5    | 107,751 0                               | 0 0 1 21 1-51  | 32455.599                            | 3080.2370                   | 3.902E+02  | 1.30E-17                 | 1.711E+05                     | 1.41290E+00        | 120    |
| 1-5    | 83,920 -                                | 0 0 2 11 2-51  | 32457.901                            | 3080.0117                   | 2.647E+02  | 2.50E-17                 | 2.64E+05                      | 1.65015E+00        | 121    |
| 2-5    | 83,920 -                                | 0 0 1 11 2-51  | 32459.566                            | 3079.9560                   | 2.233E+03  | 7.30E-17                 | 5.15E+05                      | 6.25111E+00        | 122    |
| 5-5    | 0,000 -                                 | 0 0 2 11 1-51  | 32474.170                            | 3079.4762                   | 1.369E+03  | 6.47E-17                 | 5.73E+05                      | 1.56447E+00        | 123    |
| 1-5    | 0,000 -                                 | 0 0 1 11 1-51  | 32474.523                            | 3079.4420                   | 1.961E+03  | 6.41E-17                 | 4.10E+05                      | 2.24021E+00        | 124    |
| 3-5    | 209,061 0                               | 0 0 2 21 2-51  | 32489.304                            | 3077.0346                   | 3.472E+02  | 1.13E-17                 | 2.50E+05                      | 2.27273E+00        | 125    |
| 3-5    | 429,450 0                               | 0 0 2 21 3-51  | 32517.473                            | 3074.3765                   | 2.090E+02  | 6.04E-10                 | 2.31E+05                      | 3.20653E+00        | 126    |
| 15-5   | 4371,365 -                              | 0 0 2 211 6-51 | 32531.710                            | 3073.0310                   | 4.205E+00  | 1.37E-27                 | 2.69E+05                      | 1.42637E+01        | 127    |
| 5-5    | 600,100 -                               | 0 0 2 21 4-51  | 32540.433                            | 3072.2072                   | 9.300E+01  | 3.04E-10                 | 2.490E+05                     | 6.10173E+00        | 129    |
| 1-5    | 0,000 -                                 | 0 0 2 11 1-51  | 32541.901                            | 3072.0646                   | 5.775E+02  | 2.00E-17                 | 1.00E+05                      | 9.00002E-01        | 124    |
| 2-5    | 0,000 -                                 | 0 0 1 11 1-51  | 32542.400                            | 3072.0131                   | 5.771E+02  | 1.007E-17                | 0.801E+04                     | 6.62669E-01        | 130    |
| 14-5   | 3061,676 0                              | 0 0 2 211 3-51 | 32551.652                            | 3071.1403                   | 9.616E-07  | 3.14E-26                 | 2.71E+05                      | 1.32577E+01        | 131    |
| 6-5    | 024,525 0                               | 0 0 2 21 5-51  | 32558.679                            | 3070.4055                   | 3.110E+01  | 1.01E-10                 | 2.62E+05                      | 5.17021E+00        | 132    |
| 2-5    | 03,719 0                                | 0 0 2 11 2-51  | 32559.631                            | 3070.3956                   | 6.715E+02  | 2.19E-17                 | 1.557E+05                     | 1.27305E+00        | 133    |
| 3-5    | 03,719 0                                | 0 0 1 11 2-51  | 32560.452                            | 3070.3162                   | 0.076E+02  | 2.64E-17                 | 1.40E+05                      | 1.54040E+00        | 134    |
| 15-5   | 4341,046 -                              | 0 0 2 1015-51  | 32561.229                            | 3070.2450                   | 2.396E+09  | 7.037E-29                | 1.271E+04                     | 6.77930E-01        | 135    |
| 13-5   | 3344,522 -                              | 0 0 2 2012-51  | 32567.242                            | 3069.6780                   | 1.795E-05  | 5.071E-25                | 2.74E+05                      | 1.22503E+01        | 136    |
| 7-5    | 1077,054 -                              | 0 0 2 21 6-51  | 32572.405                            | 3069.1040                   | 0.056E+00  | 2.435E-19                | 2.717E+05                     | 6.18407E+00        | 137    |
| 3-5    | 201,922 -                               | 0 0 2 11 3-51  | 32576.504                            | 3068.8053                   | 3.474E+02  | 1.130E-17                | 1.22E+05                      | 1.34301E+00        | 139    |
| 4-5    | 201,922 -                               | 0 0 1 11 3-51  | 32577.557                            | 3068.7061                   | 6.476E+02  | 2.11E-17                 | 1.031E+05                     | 2.52505E+00        | 139    |
| 12-5   | 2000,525 0                              | 0 0 2 2011-51  | 32570.555                            | 3068.6120                   | 2.721E-04  | 0.70E-24                 | 2.79E+05                      | 1.12410E+01        | 140    |

|      |      |          |   |   |         |            |           |           |           |            |             |     |
|------|------|----------|---|---|---------|------------|-----------|-----------|-----------|------------|-------------|-----|
| 8.5  | 7.5  | 1367.617 | R | 2 | 20      | 7.51       | 3060.2859 | 1.620E+60 | 5.32E-20  | 2.77E+05   | 7.19504E+00 | 161 |
| 16.5 | 16.5 | 2010.759 | R | 0 | 2       | 1016.51    | 3060.2339 | 6.237E-60 | 2.03E-27  | 2.04E+04   | 7.01104E-01 | 162 |
| 11.5 | 10.5 | 2450.279 | R | 2 | 1010.51 | 3067.0436  | 3067.0436 | 3.337E-60 | 1.09E-22  | 2.01E+05   | 1.02315E+01 | 163 |
| 15.5 | 14.5 | 3010.759 | R | 1 | 1016.51 | 32505.945  | 3067.9126 | 1.190E-06 | 3.09E-26  | 7.61E+05   | 1.39000E+01 | 164 |
| 9.5  | 9.5  | 1693.290 | R | 2 | 21      | 9.51       | 3067.7010 | 2.596E-01 | 0.691E-21 | 2.004E+05  | 0.20015E+00 | 165 |
| 10.5 | 9.5  | 2056.393 | R | 2 | 21      | 9.51       | 3067.6670 | 3.290E-02 | 1.070E-21 | 2.010E+05  | 0.22020E+00 | 166 |
| 4.5  | 4.5  | 355.105  | R | 0 | 2       | 11         | 3067.3626 | 1.350E+02 | 4.610E-10 | 9.577E+04  | 1.31733E+00 | 167 |
| 5.5  | 4.5  | 355.105  | R | 1 | 11      | 6.51       | 3067.2410 | 3.615E+02 | 1.10E-17  | 2.137E+05  | 3.55940E+00 | 168 |
| 13.5 | 13.5 | 3311.902 | R | 0 | 2       | 1013.51    | 3066.6130 | 1.339E-06 | 6.37E-26  | 1.694E+04  | 7.00641E-01 | 169 |
| 14.5 | 13.5 | 3311.902 | R | 1 | 1013.51 | 32603.023  | 3066.3109 | 2.254E-05 | 7.37E-25  | 2.644E+05  | 1.29624E+01 | 170 |
| 5.5  | 5.5  | 543.575  | R | 0 | 2       | 11         | 3066.1100 | 6.111E+01 | 1.364E-10 | 7.527E+04  | 1.25109E+00 | 171 |
| 6.5  | 5.5  | 543.575  | R | 1 | 11      | 5.51       | 3065.9766 | 1.499E+02 | 4.90E-10  | 2.35E+05   | 4.61126E+00 | 172 |
| 12.5 | 12.5 | 2046.009 | R | 0 | 2       | 1012.51    | 3065.3710 | 2.365E-05 | 7.73E-25  | 1.97E+04   | 7.70527E-01 | 173 |
| 6.5  | 6.5  | 767.650  | R | 0 | 2       | 11         | 3065.1120 | 9.965E+00 | 3.25E-10  | 5.90E+04   | 1.17227E+00 | 174 |
| 13.5 | 12.5 | 2046.009 | R | 1 | 1012.51 | 32616.012  | 3065.0479 | 3.677E-01 | 1.137E-23 | 2.697E+05  | 1.87355E+01 | 175 |
| 7.5  | 6.5  | 767.650  | R | 1 | 11      | 6.51       | 3064.9492 | 4.754E+01 | 1.95E-10  | 2.50E+05   | 5.67107E+00 | 176 |
| 11.5 | 11.5 | 2413.613 | R | 0 | 2       | 1011.51    | 3064.4942 | 3.420E-04 | 1.11E-23  | 2.317E+04  | 0.30010E-01 | 177 |
| 7.5  | 7.5  | 1026.730 | R | 0 | 2       | 11         | 3064.3741 | 1.942E+00 | 6.35E-06  | 1.0932E+00 | 1.0932E+00  | 178 |
| 12.5 | 11.5 | 2413.613 | R | 1 | 1011.51 | 32625.137  | 3064.2305 | 4.346E-03 | 1.621E-22 | 2.710E+05  | 1.09640E+01 | 179 |
| 8.5  | 7.5  | 1026.730 | R | 1 | 11      | 7.51       | 3064.1900 | 1.176E+01 | 3.04E-19  | 2.604E+05  | 6.72057E+00 | 180 |
| 10.5 | 10.5 | 2015.036 | R | 0 | 2       | 1010.51    | 3063.9710 | 4.656E-03 | 1.32E-22  | 2.74E+04   | 0.91565E-01 | 181 |
| 0.5  | 0.5  | 1321.252 | R | 0 | 2       | 11         | 3063.9256 | 3.055E-01 | 9.90E-21  | 3.95E+04   | 1.01913E+00 | 182 |
| 9.5  | 9.5  | 1650.790 | R | 1 | 2       | 11         | 3063.7854 | 3.094E-02 | 1.27E-21  | 3.27E+04   | 4.51013E-01 | 183 |
| 11.5 | 10.5 | 2015.036 | R | 1 | 1010.51 | 32628.510  | 3063.7266 | 4.300E-02 | 1.632E-21 | 2.72E+05   | 9.06003E+00 | 184 |
| 9.5  | 0.5  | 1321.252 | R | 1 | 11      | 0.51       | 3063.565  | 2.293E+00 | 7.49E-20  | 2.671E+05  | 7.7070E+00  | 185 |
| 10.5 | 9.5  | 1650.790 | R | 1 | 11      | 9.51       | 3063.5600 | 3.545E-01 | 1.15E-20  | 2.707E+05  | 0.02700E+00 | 186 |
| 2.5  | 1.5  | 856      | S | 2 | 11      | 1.51       | 3062.5260 | 1.633E+02 | 5.34E-10  | 2.30E+04   | 1.07007E-01 | 187 |
| 3.5  | 2.5  | 83.920   | S | 2 | 11      | 2.51       | 3057.7209 | 1.570E+02 | 5.13E-10  | 2.74E+04   | 2.90634E-01 | 188 |
| 4.5  | 3.5  | 202.370  | S | 2 | 11      | 3.51       | 3053.9544 | 0.567E+01 | 2.03E-10  | 2.56E+04   | 3.00030E-01 | 189 |
| 5.5  | 4.5  | 355.900  | S | 2 | 11      | 4.51       | 3060.5704 | 3.695E+01 | 1.20E-10  | 2.22E+04   | 3.63319E-01 | 190 |
| 6.5  | 5.5  | 546.009  | S | 2 | 11      | 5.51       | 3060.3101 | 1.160E+01 | 3.01E-19  | 1.07E+04   | 3.59696E-01 | 191 |
| 7.5  | 6.5  | 769.216  | S | 2 | 11      | 6.51       | 3060.3740 | 2.905E+00 | 9.69E-26  | 1.56E+04   | 3.07219E-01 | 192 |
| 0.5  | 7.5  | 1029.092 | S | 2 | 11      | 7.51       | 3036.7331 | 5.74E-01  | 1.004E-20 | 1.31E+04   | 3.31653E-01 | 193 |
| 9.5  | 0.5  | 1324.291 | S | 2 | 11      | 0.51       | 3033.6317 | 9.217E-02 | 3.014E-21 | 1.11E+04   | 3.19300E-01 | 194 |
| 10.5 | 9.5  | 1656.577 | S | 2 | 11      | 9.51       | 3030.4901 | 1.109E-02 | 3.00E-22  | 9.694E+03  | 2.99663E-01 | 195 |
| 11.5 | 10.5 | 2019.633 | S | 2 | 1010.51 | 33016.279  | 3027.9254 | 1.263E-03 | 4.07E-23  | 0.16E+03   | 2.05026E-01 | 196 |
| 12.5 | 11.5 | 2419.001 | S | 2 | 1011.51 | 33039.999  | 3025.9254 | 1.061E-04 | 3.07E-24  | 7.039E+03  | 2.71673E-01 | 197 |
| 13.5 | 12.5 | 2052.095 | S | 2 | 1012.51 | 33023.9007 | 3023.9007 | 7.377E-06 | 2.01E-25  | 6.10E+03   | 2.59626E-01 | 198 |
| 14.5 | 13.5 | 3319.355 | S | 2 | 1013.51 | 33023.974  | 3022.6651 | 4.200E-07 | 1.37E-26  | 5.39E+03   | 2.64029E-01 | 199 |
| 15.5 | 14.5 | 3019.156 | S | 2 | 1014.51 | 33003.914  | 3021.7365 | 1.965E-08 | 6.62E-20  | 4.607E+03  | 2.39107E-01 | 200 |

THE INTEGRATED INTENSITY FOR THE BAND IS 2.79600E+04 CM-2 ATM-1 AT T = 240.0 K OR 9.13039E-16 CPM/MELECM



Table 9. Line parameters for the  $A^1\Sigma^+ - X^1\Pi(g)$  OH band at 4607K.

| $J'$ | $J''$ | Lower energy<br>vacuum $\text{cm}^{-1}$ | Transition    | Frequency<br>vacuum $\text{cm}^{-1}$ | Wavelength<br>STP angstroms | Intensity<br>$\text{cm}^{-2}\text{-atm}^{-1}$ | Intensity<br>$\text{cm}/\text{molecule}$ | Einstein A<br>$\text{sec}^{-1}$ | Line<br>strength | Member |
|------|-------|---|---------------|--------------------------------------|-----------------------------|---|--|---------------------------------|------------------|--------|
| 39.5 | 46.5  | 2699.529                                | 0 P 1 2190.51 | 27339.521                            | 3656.6660                   | 3.209E-06                                     | 2.019E-24                                | 6.67E+01                        | 1.56670E-01      | 1      |
| 38.5 | 39.5  | 2500.074                                | 0 P 1 2139.51 | 27530.904                            | 3631.2320                   | 6.342E-06                                     | 3.979E-24                                | 9.70E+01                        | 1.53296E-01      | 2      |
| 37.5 | 30.5  | 24796.104                               | 0 P 1 2130.51 | 27716.057                            | 3606.0030                   | 1.165E-05                                     | 7.170E-24                                | 1.314E+02                       | 1.52320E-01      | 3      |
| 36.5 | 37.5  | 23770.737                               | 0 P 1 2137.51 | 27897.476                            | 3583.5300                   | 1.959E-05                                     | 1.220E-23                                | 1.677E+02                       | 1.51573E-01      | 4      |
| 35.5 | 36.5  | 22664.637                               | 0 P 1 2136.51 | 28073.156                            | 3561.1017                   | 3.230E-05                                     | 2.024E-23                                | 2.073E+02                       | 1.51026E-01      | 5      |
| 34.5 | 35.5  | 21656.088                               | 0 P 1 2135.51 | 28246.107                            | 3539.5400                   | 5.103E-05                                     | 3.249E-23                                | 2.503E+02                       | 1.50729E-01      | 6      |
| 33.5 | 48.5  | 20910.107                               | 0 P 2 2140.51 | 28257.590                            | 3537.0601                   | 0.005E-04                                     | 5.563E-22                                | 1.954E+04                       | 4.09727E-01      | 7      |
| 40.5 | 40.5  | 26910.107                               | 0 P 2 2140.51 | 28263.694                            | 3537.0970                   | 7.110E-06                                     | 4.463E-24                                | 1.520E+02                       | 4.29096E-01      | 8      |
| 33.5 | 34.5  | 2622.193                                | 0 P 1 2134.51 | 28410.042                            | 3510.7769                   | 0.103E-05                                     | 5.070E-23                                | 2.950E+02                       | 1.50408E-01      | 9      |
| 30.5 | 39.0  | 25037.352                               | 0 P 2 2139.51 | 28445.624                            | 3514.4761                   | 1.724E-03                                     | 1.033E-21                                | 2.013E+04                       | 3.39024E-01      | 10     |
| 39.5 | 39.5  | 25037.352                               | 0 P 1 2139.51 | 28451.690                            | 3513.7239                   | 1.653E-03                                     | 1.030E-21                                | 2.623E+02                       | 5.26730E-01      | 11     |
| 39.5 | 46.5  | 25010.569                               | 0 P 1 2140.51 | 28470.401                            | 3511.4057                   | 1.240E-03                                     | 7.967E-22                                | 2.007E+04                       | 4.11422E-01      | 12     |
| 32.5 | 33.5  | 19611.744                               | 0 P 1 2133.51 | 28573.369                            | 3490.7612                   | 1.255E-04                                     | 7.065E-23                                | 3.400E+02                       | 1.50014E-01      | 13     |
| 37.5 | 30.5  | 24766.199                               | 0 P 2 2130.51 | 28626.016                            | 3492.2200                   | 3.056E-03                                     | 1.910E-21                                | 3.705E+04                       | 3.09915E-01      | 14     |
| 30.5 | 30.5  | 24766.199                               | 0 P 1 2130.51 | 28632.060                            | 3491.4916                   | 3.234E-05                                     | 2.027E-23                                | 3.022E+02                       | 5.24950E-01      | 15     |
| 30.5 | 39.5  | 24747.204                               | 0 P 1 1139.51 | 28651.775                            | 3489.1056                   | 2.435E-03                                     | 1.539E-21                                | 2.007E+04                       | 4.01540E-01      | 16     |
| 31.5 | 32.5  | 18610.424                               | 0 P 2 2137.51 | 28732.007                            | 3479.4430                   | 1.909E-04                                     | 1.194E-22                                | 4.043E+02                       | 1.51232E-01      | 17     |
| 36.5 | 37.5  | 23705.526                               | 0 P 2 2137.51 | 28801.537                            | 3471.0466                   | 5.107E-03                                     | 3.207E-21                                | 4.627E+04                       | 3.00001E-01      | 18     |
| 37.5 | 37.5  | 23705.526                               | 0 P 1 2137.51 | 28807.515                            | 3470.3227                   | 5.005E-05                                     | 3.639E-23                                | 5.114E+02                       | 5.23001E-01      | 19     |
| 37.5 | 30.5  | 23600.672                               | 0 P 1 1130.51 | 28826.569                            | 3460.0228                   | 4.334E-03                                     | 2.710E-21                                | 3.000E+04                       | 1.51915E-01      | 20     |
| 30.5 | 31.5  | 17637.220                               | 0 P 1 2131.51 | 28806.947                            | 3460.7799                   | 2.075E-04                                     | 1.002E-22                                | 4.670E+02                       | 1.51915E-01      | 21     |
| 35.5 | 36.5  | 22656.237                               | 0 P 2 2136.51 | 28970.010                            | 3450.0567                   | 0.239E-03                                     | 5.164E-21                                | 5.540E+04                       | 3.70001E-01      | 22     |
| 36.5 | 36.5  | 22656.237                               | 0 P 1 2136.51 | 28975.976                            | 3450.1683                   | 9.007E-03                                     | 6.197E-21                                | 6.510E+02                       | 5.23201E-01      | 23     |
| 36.5 | 37.5  | 22637.036                               | 0 P 1 1137.51 | 28995.177                            | 3447.0615                   | 7.229E-03                                     | 4.533E-21                                | 4.743E+04                       | 3.01756E-01      | 24     |
| 29.5 | 30.5  | 16075.095                               | 0 P 1 2130.51 | 29030.602                            | 3442.7290                   | 4.200E-04                                     | 2.600E-22                                | 5.302E+02                       | 1.52079E-01      | 25     |
| 40.5 | 40.5  | 26949.579                               | 0 Q 2 2140.51 | 29120.465                            | 3433.0269                   | 1.100E-02                                     | 7.000E-22                                | 2.573E+04                       | 0.16577E-01      | 26     |
| 34.5 | 35.5  | 21619.256                               | 0 P 2 2135.51 | 29132.621                            | 3431.5044                   | 1.209E-02                                     | 1.000E-22                                | 6.563E+04                       | 3.60155E-01      | 27     |
| 35.5 | 35.5  | 21619.256                               | 0 P 1 2135.51 | 29138.537                            | 3430.0977                   | 1.674E-04                                     | 1.010E-22                                | 9.670E+02                       | 5.23422E-01      | 28     |
| 35.5 | 36.5  | 21599.090                               | 0 P 1 1136.51 | 29157.024                            | 3420.6199                   | 1.640E-02                                     | 7.260E-21                                | 5.717E+04                       | 3.71074E-01      | 29     |
| 28.5 | 29.5  | 15731.031                               | 0 P 2 2134.51 | 29106.542                            | 3425.2505                   | 6.310E-04                                     | 3.960E-22                                | 6.100E+02                       | 1.54120E-01      | 30     |
| 33.5 | 34.5  | 20595.523                               | 0 P 2 2134.51 | 29209.614                            | 3413.2004                   | 1.950E-02                                     | 1.227E-20                                | 7.535E+04                       | 3.50222E-01      | 31     |
| 34.5 | 34.5  | 20595.523                               | 0 P 1 2134.51 | 29295.673                            | 3412.5177                   | 2.507E-04                                     | 1.622E-22                                | 9.670E+02                       | 5.24252E-01      | 32     |
| 39.5 | 39.5  | 25060.074                               | 0 Q 2 2139.51 | 29307.631                            | 3411.1921                   | 2.545E-03                                     | 1.599E-21                                | 3.000E+04                       | 7.96633E-01      | 33     |
| 40.5 | 39.5  | 25060.074                               | 0 R 1 2139.51 | 29313.727                            | 3410.3927                   | 6.302E-06                                     | 1.000E-24                                | 1.000E+02                       | 2.95112E-01      | 34     |
| 34.5 | 35.5  | 20575.990                               | 0 P 1 1135.51 | 29314.990                            | 3410.2440                   | 1.401E-02                                     | 1.132E-20                                | 6.720E+04                       | 3.61900E-01      | 35     |
| 39.5 | 40.5  | 25455.390                               | 0 P 2 1140.51 | 29323.316                            | 3409.6263                   | 1.107E-05                                     | 6.910E-24                                | 2.625E+04                       | 3.52704E-01      | 36     |
| 40.5 | 40.5  | 25095.390                               | 0 Q 1 1140.51 | 29326.412                            | 3409.9175                   | 1.503E-03                                     | 9.925E-22                                | 1.079E+04                       | 0.13570E-01      | 37     |
| 27.5 | 28.5  | 14006.007                               | 0 P 1 2120.51 | 29331.526                            | 3400.7231                   | 9.213E-04                                     | 5.775E-22                                | 7.059E+02                       | 1.55602E-01      | 38     |
| 32.5 | 33.5  | 19505.991                               | 0 P 2 2133.51 | 29441.240                            | 3395.0205                   | 4.019E-02                                     | 1.043E-20                                | 0.590E+04                       | 3.40203E-01      | 39     |
| 33.5 | 33.5  | 19505.991                               | 0 P 1 2133.51 | 29447.044                            | 3394.9522                   | 4.019E-04                                     | 2.533E-22                                | 1.145E+03                       | 5.25799E-01      | 40     |
| 33.5 | 36.5  | 19566.207                               | 0 P 1 1130.51 | 29466.747                            | 3392.6022                   | 2.733E-02                                     | 3.713E-20                                | 7.713E+04                       | 3.52077E-01      | 41     |
| 26.5 | 27.5  | 13000.997                               | 0 Q 2 2127.51 | 29473.450                            | 3391.9059                   | 1.320E-03                                     | 3.052E-22                                | 0.024E+02                       | 1.57507E-01      | 42     |
| 30.5 | 30.5  | 24796.104                               | 0 Q 2 2130.51 | 29406.793                            | 3390.3755                   | 4.049E-03                                     | 3.052E-21                                | 6.159E+04                       | 7.74603E-01      | 43     |
| 30.5 | 36.5  | 24796.104                               | 0 R 1 2130.51 | 29492.066                            | 3309.6774                   | 1.394E-05                                     | 0.767E-24                                | 1.726E+02                       | 2.95702E-01      | 44     |
| 30.5 | 39.5  | 24703.345                               | 0 P 2 1139.51 | 29499.632                            | 3300.0939                   | 2.195E-05                                     | 1.374E-23                                | 2.767E+02                       | 3.52570E-01      | 45     |
| 30.5 | 30.5  | 24703.345                               | 0 Q 1 1139.51 | 29505.705                            | 3300.2023                   | 3.522E-03                                     | 1.252E-21                                | 4.410E+04                       | 7.93610E-01      | 46     |
| 31.5 | 32.5  | 18591.624                               | 0 P 2 2132.51 | 29507.766                            | 3370.0956                   | 4.327E-02                                     | 2.712E-20                                | 9.645E+04                       | 3.30336E-01      | 47     |

|      |      |           |   |   |   |         |           |           |           |           |           |             |     |
|------|------|-----------|---|---|---|---------|-----------|-----------|-----------|-----------|-----------|-------------|-----|
| 32.5 | 32.5 | 10591.624 | 0 | 0 | 1 | 2132.53 | 29593.640 | 3370.4514 | 6.221E-04 | 3.099E-22 | 1.345E+03 | 5.20099E-01 | 69  |
| 25.5 | 26.5 | 13016.966 | 0 | 0 | 1 | 2126.53 | 29612.505 | 3375.0730 | 1.902E-03 | 1.182E-21 | 9.348E+02 | 1.50034E-01 | 69  |
| 32.5 | 33.5 | 10571.723 | 0 | 0 | 1 | 1133.53 | 29613.306 | 3375.0837 | 4.005E-02 | 2.940E-20 | 6.790E+04 | 1.62172E-01 | 69  |
| 37.5 | 37.5 | 23734.737 | 0 | 0 | 2 | 2137.53 | 29650.270 | 3370.7716 | 0.534E-03 | 5.349E-21 | 0.040E+04 | 7.94727E-01 | 51  |
| 30.5 | 37.5 | 23726.737 | 0 | 0 | 1 | 2137.53 | 29664.322 | 3370.0049 | 2.605E-05 | 1.603E-21 | 2.467E+02 | 2.96017E-01 | 52  |
| 37.5 | 30.5 | 23721.729 | 0 | 0 | 1 | 1130.53 | 29671.206 | 3369.2939 | 3.974E-05 | 2.493E-23 | 3.730E+02 | 1.52042E-01 | 53  |
| 30.5 | 30.5 | 23721.729 | 0 | 0 | 1 | 1130.53 | 29677.330 | 3360.6877 | 6.050E-03 | 4.293E-21 | 6.270E+04 | 7.79674E-01 | 54  |
| 30.5 | 31.5 | 17613.392 | 0 | 0 | 2 | 2131.53 | 29729.391 | 3362.7004 | 2.207E-02 | 3.940E-20 | 1.079E+05 | 3.20302E-01 | 55  |
| 31.5 | 31.5 | 17613.392 | 0 | 0 | 1 | 2131.53 | 29735.030 | 3362.6699 | 9.467E-04 | 5.914E-22 | 1.569E+03 | 5.31109E-01 | 55  |
| 24.5 | 25.5 | 12154.073 | 0 | 0 | 1 | 2125.53 | 29740.962 | 3360.5030 | 2.691E-03 | 1.647E-21 | 1.030E+03 | 1.62469E-01 | 57  |
| 31.5 | 32.5 | 17593.290 | 0 | 0 | 1 | 1132.53 | 29755.140 | 3359.7905 | 5.961E-02 | 3.709E-20 | 9.060E+04 | 3.32260E-01 | 59  |
| 36.5 | 36.5 | 22604.637 | 0 | 0 | 2 | 2136.53 | 29822.396 | 3352.2211 | 1.416E-02 | 0.077E-21 | 9.970E+04 | 7.34762E-01 | 59  |
| 37.5 | 36.5 | 22604.637 | 0 | 0 | 1 | 2136.53 | 29820.436 | 3351.7459 | 6.775E-05 | 2.933E-23 | 3.277E+02 | 2.90234E-01 | 60  |
| 36.5 | 37.5 | 22671.646 | 0 | 0 | 2 | 1137.53 | 29935.507 | 3350.7196 | 6.014E-05 | 4.274E-23 | 4.709E+02 | 3.53513E-01 | 61  |
| 37.5 | 37.5 | 22671.646 | 0 | 0 | 1 | 1137.53 | 29945.595 | 3350.0644 | 1.196E-02 | 7.690E-21 | 0.100E+04 | 0.100E+04   | 62  |
| 29.5 | 30.5 | 11692.271 | 0 | 0 | 2 | 2130.53 | 29966.335 | 3347.2091 | 9.002E-02 | 5.643E-20 | 1.109E+05 | 3.10420E-01 | 62  |
| 30.5 | 30.5 | 11692.271 | 0 | 0 | 1 | 2130.53 | 29971.096 | 3346.6661 | 1.421E-03 | 0.900E-22 | 1.017E+03 | 5.39119E-01 | 64  |
| 23.5 | 24.5 | 11315.683 | 0 | 0 | 1 | 2124.53 | 29982.546 | 3345.6732 | 3.703E-03 | 2.318E-21 | 1.170E+03 | 1.65919E-01 | 65  |
| 30.5 | 31.5 | 11631.946 | 0 | 0 | 1 | 1131.53 | 29992.221 | 3344.3904 | 0.645E-02 | 5.419E-20 | 1.100E+05 | 3.22349E-01 | 66  |
| 35.5 | 35.5 | 21646.000 | 0 | 0 | 2 | 2135.53 | 29979.629 | 3334.6604 | 2.263E-02 | 1.410E-20 | 1.197E+05 | 7.10791E-01 | 67  |
| 35.5 | 35.5 | 21646.000 | 0 | 0 | 1 | 2135.53 | 29985.404 | 3333.9970 | 0.091E-05 | 5.070E-23 | 4.165E+02 | 3.00054E-01 | 68  |
| 35.5 | 36.5 | 21433.810 | 0 | 0 | 2 | 1136.53 | 29992.029 | 3333.1716 | 1.126E-04 | 7.095E-23 | 5.934E+02 | 3.56011E-01 | 69  |
| 20.5 | 29.5 | 13709.237 | 0 | 0 | 2 | 2129.53 | 29990.795 | 3332.5090 | 1.275E-01 | 7.909E-20 | 1.300E+05 | 3.00440E-01 | 70  |
| 36.5 | 36.5 | 21633.810 | 0 | 0 | 1 | 1136.53 | 29990.795 | 3332.5090 | 1.977E-02 | 1.239E-21 | 1.016E+05 | 7.37070E-01 | 71  |
| 29.5 | 29.5 | 15709.237 | 0 | 0 | 1 | 2129.53 | 30064.240 | 3331.9017 | 2.310E-03 | 1.302E-21 | 2.092E+03 | 5.39924E-01 | 72  |
| 22.5 | 23.5 | 10500.267 | 0 | 0 | 1 | 2123.53 | 30033.654 | 3330.0644 | 5.250E-03 | 3.294E-21 | 1.339E+03 | 1.69013E-01 | 73  |
| 29.5 | 30.5 | 15600.670 | 0 | 0 | 1 | 1130.53 | 30024.026 | 3329.6194 | 1.231E-01 | 7.717E-20 | 1.230E+05 | 3.12430E-01 | 74  |
| 27.5 | 28.5 | 16705.263 | 0 | 0 | 2 | 2120.53 | 30126.944 | 3310.3330 | 1.777E-01 | 1.114E-19 | 1.627E+05 | 2.90669E-01 | 75  |
| 34.5 | 34.5 | 21622.193 | 0 | 0 | 2 | 2134.53 | 30129.604 | 3310.0312 | 3.497E-02 | 2.192E-20 | 1.399E+05 | 6.06013E-01 | 76  |
| 20.5 | 20.5 | 14745.263 | 0 | 0 | 1 | 2120.53 | 30122.310 | 3317.7420 | 3.090E-03 | 1.937E-21 | 2.397E+03 | 5.65070E-01 | 77  |
| 35.5 | 36.5 | 21622.193 | 0 | 0 | 1 | 2134.53 | 30135.600 | 3317.3790 | 1.313E-04 | 0.227E-23 | 5.090E+02 | 3.02297E-01 | 78  |
| 21.5 | 22.5 | 9709.602  | 0 | 0 | 1 | 2122.53 | 30142.147 | 3316.6592 | 7.252E-03 | 4.546E-21 | 1.517E+03 | 1.73006E-01 | 79  |
| 35.5 | 35.5 | 20600.506 | 0 | 0 | 2 | 1135.53 | 30143.291 | 3316.5334 | 1.067E-04 | 1.134E-20 | 7.109E+02 | 3.60159E-01 | 80  |
| 35.5 | 35.5 | 20600.506 | 0 | 0 | 1 | 1135.53 | 30149.207 | 3315.0026 | 3.144E-02 | 1.974E-20 | 1.216E+05 | 7.13303E-01 | 81  |
| 23.5 | 29.5 | 14764.634 | 0 | 0 | 1 | 1129.53 | 30153.139 | 3315.6502 | 1.733E-01 | 1.006E-19 | 1.330E+05 | 3.02305E-01 | 82  |
| 40.5 | 39.5 | 25437.352 | 0 | 0 | 2 | 2134.53 | 30232.641 | 3306.7312 | 0.706E-04 | 5.657E-22 | 1.529E+04 | 3.91496E-01 | 83  |
| 26.5 | 27.5 | 13001.320 | 0 | 0 | 2 | 2127.53 | 30250.955 | 3304.7292 | 2.442E-01 | 1.530E-19 | 1.549E+05 | 2.00479E-01 | 84  |
| 40.5 | 46.5 | 25010.569 | 0 | 0 | 2 | 1160.53 | 30251.424 | 3304.6761 | 0.926E-06 | 5.599E-24 | 1.554E+02 | 4.39496E-01 | 85  |
| 27.5 | 27.5 | 13001.320 | 0 | 0 | 1 | 2127.53 | 30256.213 | 3306.1550 | 4.446E-03 | 2.038E-21 | 2.737E+03 | 5.52434E-01 | 86  |
| 20.5 | 21.5 | 0764.563  | 0 | 0 | 1 | 2121.53 | 30260.236 | 3302.0425 | 9.090E-03 | 6.204E-21 | 1.720E+03 | 1.77044E-01 | 87  |
| 33.5 | 33.5 | 19611.744 | 0 | 0 | 2 | 2132.53 | 30273.392 | 3302.2600 | 5.206E-02 | 3.313E-20 | 1.597E+05 | 6.74027E-01 | 89  |
| 27.5 | 20.5 | 13060.205 | 0 | 0 | 1 | 1120.53 | 30277.329 | 3301.0506 | 2.402E-01 | 1.504E-19 | 1.459E+05 | 2.92574E-01 | 89  |
| 34.5 | 33.5 | 19611.744 | 0 | 0 | 1 | 2133.53 | 30279.251 | 3301.6409 | 2.099E-04 | 1.319E-22 | 6.162E+02 | 3.04904E-01 | 90  |
| 33.5 | 34.5 | 19597.902 | 0 | 0 | 2 | 1134.53 | 30207.236 | 3300.7707 | 2.030E-04 | 1.773E-22 | 0.521E+02 | 3.50169E-01 | 91  |
| 34.5 | 34.5 | 19597.902 | 0 | 0 | 1 | 1134.53 | 30293.374 | 3300.3322 | 4.030E-02 | 3.032E-20 | 1.616E+05 | 2.70470E-01 | 92  |
| 25.5 | 26.5 | 12990.371 | 0 | 0 | 2 | 2126.53 | 30370.941 | 3291.6646 | 3.321E-01 | 2.000E-19 | 1.609E+05 | 2.70470E-01 | 93  |
| 26.5 | 26.5 | 12990.371 | 0 | 0 | 1 | 2126.53 | 30376.124 | 3291.1133 | 6.430E-03 | 4.030E-21 | 3.113E+03 | 5.60204E-01 | 94  |
| 19.5 | 20.5 | 0206.027  | 0 | 0 | 1 | 2120.53 | 30391.910 | 3209.0009 | 1.341E-02 | 0.499E-21 | 1.960E+03 | 1.92606E-01 | 95  |
| 26.5 | 27.5 | 12974.943 | 0 | 0 | 1 | 1127.53 | 30397.552 | 3290.7912 | 3.201E-01 | 2.090E-19 | 1.500E+05 | 2.02630E-01 | 96  |
| 39.5 | 30.5 | 24766.199 | 0 | 0 | 2 | 2130.53 | 30429.507 | 3207.6903 | 1.070E-03 | 1.197E-21 | 2.449E+04 | 3.01609E-01 | 97  |
| 32.5 | 32.5 | 14616.429 | 0 | 0 | 2 | 2132.53 | 30410.009 | 3207.6903 | 7.065E-02 | 4.936E-20 | 1.010E+05 | 6.50032E-01 | 98  |
| 33.5 | 32.5 | 14616.429 | 0 | 0 | 1 | 2132.53 | 30416.665 | 3246.7310 | 3.207E-04 | 2.000E-22 | 7.363E+02 | 3.00167E-01 | 99  |
| 32.5 | 32.5 | 14602.331 | 0 | 0 | 2 | 1133.53 | 30424.950 | 3205.0841 | 4.302E-04 | 2.707E-22 | 1.609E+03 | 3.60670E-01 | 100 |

Table 3 (Contd.)

| J' J''    | Lower energy vacuum cm <sup>-1</sup> | Transition    | Frequency vacuum cm <sup>-1</sup> | Wavelength STP angstroms | Intensity cm <sup>-2</sup> atm <sup>-1</sup> | Intensity cm/molecule | Einstein sec <sup>-1</sup> | Line strength | Number |
|-----------|--------------------------------------|---------------|-----------------------------------|--------------------------|--|-----------------------|----------------------------|---------------|--------|
| 39.5 39.5 | 26747.204                            | Q 0 2 1039.51 | 30420.421                         | 3205.4567                | 2.049E-05                                    | 1.29E-23              | 2.674E-02                  | 6.20270E-01   | 104    |
| 33.5 33.5 | 16022.331                            | Q 0 1 1033.51 | 30430.703                         | 3205.2003                | 7.276E-02                                    | 4.56E-20              | 1.620E-05                  | 6.73694E-01   | 102    |
| 40.5 39.5 | 22797.204                            | Q 0 1 1039.51 | 30436.517                         | 3206.7966                | 1.220E-03                                    | 7.60E-22              | 1.950E-06                  | 1.00114E-01   | 103    |
| 24.5 25.5 | 12137.370                            | P 0 2 2025.51 | 30407.162                         | 3270.1262                | 4.449E-01                                    | 2.70E-19              | 1.700E-05                  | 2.60466E-01   | 106    |
| 25.5 25.5 | 12137.370                            | P 0 1 2025.51 | 30492.102                         | 3276.5664                | 9.134E-03                                    | 5.72E-21              | 3.539E-03                  | 5.69307E-01   | 105    |
| 10.5 19.5 | 7494.040                             | P 0 1 2019.51 | 30513.229                         | 3276.3229                | 1.001E-02                                    | 1.12E-20              | 2.232E-03                  | 1.00501E-01   | 104    |
| 25.5 26.5 | 12115.590                            | P 0 1 1026.51 | 30513.954                         | 3276.2450                | 6.433E-01                                    | 2.77E-19              | 1.704E-05                  | 2.72696E-01   | 107    |
| 31.5 31.5 | 17337.220                            | Q 0 2 2031.51 | 30542.169                         | 3273.2193                | 1.154E-01                                    | 7.23E-20              | 2.031E-05                  | 6.34027E-01   | 100    |
| 32.5 31.5 | 17637.220                            | Q 0 1 2031.51 | 30547.093                         | 3272.6049                | 5.077E-04                                    | 3.10E-22              | 0.670E-02                  | 3.11010E-01   | 109    |
| 31.5 32.5 | 17622.044                            | Q 0 2 1032.51 | 30556.545                         | 3271.6783                | 6.662E-04                                    | 4.17E-22              | 1.170E-03                  | 3.63711E-01   | 110    |
| 32.5 32.5 | 17622.044                            | Q 0 1 1032.51 | 30562.269                         | 3271.0655                | 1.077E-01                                    | 6.75E-20              | 1.034E-05                  | 6.53013E-01   | 112    |
| 30.5 37.5 | 23785.526                            | Q 0 2 2037.51 | 30577.451                         | 3269.4413                | 3.494E-53                                    | 2.19E-21              | 3.303E-04                  | 1.71711E-01   | 112    |
| 10.5 30.5 | 23086.472                            | Q 0 2 1030.51 | 30596.505                         | 3267.4052                | 4.030E-05                                    | 2.53E-23              | 3.007E-02                  | 4.37965E-01   | 113    |
| 23.5 24.5 | 11299.250                            | P 0 2 2024.51 | 30599.820                         | 3267.0717                | 5.091E-01                                    | 3.69E-19              | 1.914E-05                  | 2.50442E-01   | 116    |
| 39.5 30.5 | 23606.472                            | Q 0 1 1030.51 | 31602.570                         | 3266.7560                | 2.640E-03                                    | 1.65E-21              | 2.470E-04                  | 1.00211E-01   | 115    |
| 24.5 24.5 | 11299.250                            | P 0 1 2024.51 | 30604.517                         | 3266.5490                | 1.206E-02                                    | 0.06E-21              | 4.012E-03                  | 5.79608E-01   | 116    |
| 24.5 25.5 | 11277.107                            | P 0 1 1025.51 | 30606.060                         | 3266.1072                | 5.096E-01                                    | 3.69E-19              | 1.679E-05                  | 2.62745E-01   | 117    |
| 17.5 10.5 | 6081.055                             | Q 0 1 2010.51 | 30632.193                         | 3263.5944                | 2.390E-02                                    | 1.50E-20              | 2.557E-03                  | 1.95070E-01   | 110    |
| 30.5 30.5 | 16075.095                            | Q 0 2 2030.51 | 30667.609                         | 3259.0209                | 1.664E-01                                    | 1.04E-19              | 2.25E-05                   | 1.14010E-01   | 119    |
| 31.5 30.5 | 16075.095                            | Q 0 1 2030.51 | 30673.335                         | 3259.2280                | 7.723E-04                                    | 4.04E-22              | 1.014E-03                  | 1.16007E-01   | 120    |
| 30.5 31.5 | 16660.617                            | Q 0 2 1031.51 | 30602.365                         | 3250.2614                | 1.002E-03                                    | 6.20E-22              | 1.355E-03                  | 1.67300E-01   | 121    |
| 31.5 31.5 | 16660.617                            | Q 0 1 1031.51 | 30600.012                         | 3257.6619                | 1.571E-01                                    | 9.04E-20              | 2.059E-05                  | 3.43022E-01   | 122    |
| 22.5 23.5 | 10806.962                            | P 0 2 2023.51 | 30700.695                         | 3255.6490                | 7.409E-01                                    | 4.01E-19              | 2.035E-05                  | 2.40404E-01   | 123    |
| 23.5 23.5 | 14084.962                            | P 0 1 2023.51 | 30713.247                         | 3254.9053                | 1.792E-02                                    | 1.12E-20              | 4.546E-03                  | 5.91209E-01   | 124    |
| 23.5 24.5 | 10462.346                            | P 0 1 2024.51 | 30735.016                         | 3252.5951                | 7.760E-01                                    | 4.06E-19              | 1.957E-05                  | 2.52707E-01   | 125    |
| 37.5 36.5 | 22656.237                            | Q 0 2 2026.51 | 30736.770                         | 3252.4933                | 6.023E-03                                    | 3.77E-21              | 4.353E-04                  | 1.61013E-01   | 126    |
| 16.5 17.5 | 6157.034                             | Q 0 1 2017.51 | 30740.024                         | 3251.2191                | 3.162E-02                                    | 1.90E-20              | 2.932E-03                  | 2.02609E-01   | 127    |
| 37.5 37.5 | 22637.036                            | Q 0 2 1037.51 | 30755.979                         | 3250.4627                | 7.231E-05                                    | 4.53E-23              | 1.190E-02                  | 6.37681E-01   | 120    |
| 30.5 37.5 | 22637.036                            | Q 0 1 1037.51 | 30762.023                         | 3249.0240                | 4.090E-03                                    | 3.07E-21              | 3.632E-04                  | 1.70303E-01   | 129    |
| 29.5 29.5 | 15731.031                            | Q 0 2 2029.51 | 30707.575                         | 3247.1267                | 2.366E-01                                    | 1.40E-19              | 2.600E-05                  | 5.44794E-01   | 130    |
| 30.5 29.5 | 15731.031                            | Q 0 1 2029.51 | 30793.136                         | 3246.5403                | 1.162E-03                                    | 9.33E-22              | 1.194E-03                  | 1.20775E-01   | 131    |
| 30.5 36.5 | 15716.026                            | Q 0 2 1030.51 | 30802.500                         | 3246.5403                | 1.609E-03                                    | 9.33E-22              | 1.564E-03                  | 1.71602E-01   | 132    |
| 30.5 30.5 | 15716.026                            | Q 0 1 1030.51 | 30800.141                         | 3246.9591                | 2.254E-01                                    | 1.41E-19              | 2.207E-05                  | 6.13020E-01   | 133    |
| 21.5 22.5 | 9695.394                             | P 0 2 2022.51 | 30813.069                         | 3244.3550                | 9.106E-01                                    | 6.21E-19              | 2.157E-05                  | 2.30351E-01   | 134    |
| 22.5 22.5 | 9695.394                             | P 0 1 2022.51 | 30810.477                         | 3243.0707                | 2.672E-02                                    | 1.54E-20              | 5.146E-03                  | 6.04507E-01   | 135    |
| 22.5 23.5 | 9672.362                             | P 0 1 1023.51 | 30841.509                         | 3241.6401                | 1.006E-00                                    | 6.30E-19              | 2.002E-05                  | 2.40202E-01   | 136    |
| 15.5 16.5 | 5533.620                             | Q 0 1 2016.51 | 30863.123                         | 3239.1700                | 4.139E-02                                    | 2.59E-20              | 3.300E-03                  | 2.10069E-01   | 137    |
| 36.5 35.5 | 21619.256                            | Q 0 2 2035.51 | 30807.777                         | 3236.5925                | 9.060E-03                                    | 6.10E-21              | 5.340E-04                  | 2.10069E-01   | 139    |
| 20.5 20.5 | 14006.007                            | Q 0 2 2020.51 | 30905.022                         | 3235.1005                | 3.317E-01                                    | 2.07E-19              | 2.723E-05                  | 5.74761E-01   | 139    |
| 36.5 36.5 | 21599.050                            | Q 0 2 1036.51 | 30907.135                         | 3234.5653                | 1.220E-04                                    | 7.60E-23              | 6.620E-02                  | 4.37023E-01   | 140    |
| 29.5 20.5 | 14006.007                            | Q 0 1 2020.51 | 30907.409                         | 3234.5242                | 1.722E-03                                    | 1.07E-21              | 1.367E-03                  | 1.26157E-01   | 141    |
| 37.5 36.5 | 21599.050                            | Q 0 1 1036.51 | 30913.163                         | 3233.9366                | 0.396E-03                                    | 5.26E-21              | 4.006E-04                  | 1.60390E-01   | 142    |
| 20.5 21.5 | 9731.646                             | P 0 2 2021.51 | 30915.046                         | 3233.6530                | 1.260E-00                                    | 7.00E-19              | 2.274E-05                  | 2.20203E-01   | 143    |
| 20.5 29.5 | 14790.647                            | Q 0 2 1029.51 | 30917.303                         | 3233.6431                | 2.193E-03                                    | 1.37E-21              | 1.794E-03                  | 1.76297E-01   | 144    |
| 21.5 21.5 | 9731.646                             | P 0 1 2021.51 | 30923.303                         | 3233.1077                | 3.302E-02                                    | 2.12E-20              | 5.037E-03                  | 6.19413E-01   | 145    |
| 29.5 29.5 | 14790.647                            | Q 0 1 1029.51 | 30922.050                         | 3232.9214                | 3.105E-01                                    | 1.99E-19              | 2.519E-05                  | 5.93910E-01   | 146    |

|      |      |           |           |           |           |           |           |              |     |
|------|------|-----------|-----------|-----------|-----------|-----------|-----------|--------------|-----|
| 21.5 | 22.5 | 0907.070  | 3693.051  | 3230.7272 | 1.200E+00 | 0.074E-19 | 2.300E+03 | 2.32050E+01  | 167 |
| 16.5 | 19.5 | 6939.082  | 36975.003 | 3227.6676 | 5.360E-02 | 2.304E-20 | 3.910E+03 | 2.29794E-01  | 168 |
| 27.5 | 27.5 | 13980.997 | 31011.210 | 3223.7076 | 6.507E-01 | 7.079E-19 | 2.960E+05 | 5.56716E+01  | 169 |
| 19.5 | 20.5 | 0193.990  | 31010.510 | 3223.3665 | 1.501E+00 | 9.506E-19 | 2.394E+05 | 2.10190E+01  | 159 |
| 20.5 | 27.5 | 13980.997 | 31010.576 | 3223.1510 | 2.530E-03 | 2.304E-21 | 1.570E+03 | 3.32200E-01  | 151 |
| 20.5 | 27.5 | 0193.990  | 31010.089 | 3222.9190 | 6.507E-02 | 2.073E-20 | 6.610E+03 | 6.36194E-01  | 152 |
| 27.5 | 20.5 | 13065.249 | 31026.957 | 3222.6733 | 3.100E-03 | 1.990E-21 | 2.040E+03 | 3.01794E-01  | 153 |
| 35.5 | 34.5 | 20995.523 | 31030.725 | 3221.6421 | 1.542E-02 | 2.700E-19 | 6.200E+06 | 3.27000E+01  | 154 |
| 20.5 | 20.5 | 01905.249 | 31032.324 | 3221.5161 | 6.435E-01 | 2.700E-19 | 2.750E+05 | 5.73000E+01  | 155 |
| 20.5 | 21.5 | 0169.066  | 31042.933 | 3220.6151 | 1.624E+00 | 1.010E-10 | 2.330E+05 | 2.22000E+01  | 156 |
| 35.5 | 35.5 | 20975.990 | 31050.250 | 3219.0562 | 2.012E-04 | 1.260E-22 | 0.100E+02 | 6.30994E-01  | 157 |
| 13.5 | 14.5 | 6377.619  | 31004.603 | 3216.0096 | 6.094E-02 | 6.322E-20 | 6.540E+03 | 2.31000E-01  | 159 |
| 10.5 | 19.5 | 7403.075  | 31109.936 | 3213.0700 | 1.956E+00 | 1.224E-10 | 2.510E+05 | 2.00093E+01  | 160 |
| 19.5 | 19.5 | 7403.075  | 31114.070 | 3213.0519 | 6.153E-02 | 3.057E-20 | 7.510E+03 | 6.55605E-01  | 161 |
| 26.5 | 19.5 | 13016.966 | 31115.319 | 3212.5239 | 6.249E-01 | 3.910E-19 | 3.130E+05 | 5.31660E+01  | 162 |
| 27.5 | 26.5 | 13016.966 | 31120.567 | 3212.2011 | 6.677E-03 | 2.309E-21 | 1.010E+03 | 3.30959E-01  | 163 |
| 26.5 | 27.5 | 13000.797 | 31131.670 | 3211.2551 | 6.570E-03 | 2.070E-21 | 2.390E+03 | 3.00027E-01  | 164 |
| 27.5 | 27.5 | 13000.797 | 31136.736 | 3210.7120 | 6.693E-01 | 3.010E-19 | 2.991E+05 | 5.33054E+01  | 165 |
| 19.5 | 20.5 | 7659.105  | 31130.079 | 3210.6962 | 2.022E+00 | 1.260E-10 | 2.690E+05 | 2.32077E+01  | 166 |
| 34.5 | 33.5 | 19565.991 | 31165.006 | 3207.7097 | 2.371E-02 | 1.600E-20 | 7.310E+04 | 3.32004E+01  | 167 |
| 34.5 | 36.5 | 19566.207 | 31105.509 | 3205.6036 | 3.195E-04 | 2.062E-22 | 9.010E+02 | 6.07000E-01  | 169 |
| 35.5 | 34.5 | 19566.207 | 31191.565 | 3205.0749 | 2.130E-02 | 1.319E-20 | 3.600E+04 | 3.03043E+01  | 169 |
| 12.5 | 33.5 | 3046.059  | 31191.092 | 3205.0352 | 0.799E-02 | 5.510E-20 | 5.320E+03 | 2.03203E-01  | 170 |
| 17.5 | 30.5 | 6001.926  | 31202.100 | 3203.9776 | 2.306E+00 | 1.699E-10 | 2.630E+05 | 1.09967E+01  | 171 |
| 10.5 | 10.5 | 6901.026  | 31206.151 | 3203.5707 | 0.174E-02 | 5.123E-20 | 0.540E+03 | 6.76291E-01  | 172 |
| 25.5 | 25.5 | 12154.073 | 31210.479 | 3202.7159 | 0.606E-01 | 5.260E-19 | 3.420E+05 | 5.10590E+01  | 173 |
| 26.5 | 26.5 | 12156.073 | 31219.622 | 3202.3004 | 5.270E-03 | 3.300E-21 | 2.070E+03 | 3.66490E-01  | 174 |
| 25.5 | 26.5 | 12130.246 | 31231.100 | 3201.0106 | 6.527E-03 | 6.690E-21 | 2.650E+03 | 3.95050E-01  | 175 |
| 10.5 | 19.5 | 0776.031  | 31231.646 | 3200.9555 | 2.600E+00 | 1.550E-10 | 2.500E+05 | 2.02076E+01  | 174 |
| 26.5 | 26.5 | 12130.246 | 31236.251 | 3200.6036 | 9.264E-01 | 5.167E-19 | 3.220E+05 | 5.33007E+01  | 177 |
| 40.5 | 39.5 | 24703.145 | 31206.649 | 3195.3279 | 5.912E-06 | 3.704E-24 | 7.970E+01 | 1.06700E-01  | 179 |
| 10.5 | 17.5 | 0160.942  | 31291.320 | 3194.0509 | 2.065E+09 | 1.790E-10 | 2.740E+05 | 1.79010E+01  | 179 |
| 33.5 | 32.5 | 10501.624 | 31293.513 | 3194.6270 | 3.563E-02 | 2.233E-20 | 0.361E+04 | 3.22100E+01  | 180 |
| 17.5 | 17.5 | 0160.942  | 31295.166 | 3194.6444 | 1.070E-01 | 6.754E-20 | 9.740E+03 | 7.000164E-01 | 181 |
| 11.5 | 12.5 | 3340.000  | 31296.666 | 3194.3051 | 1.112E-01 | 6.973E-20 | 6.200E+03 | 2.56974E-01  | 182 |
| 24.5 | 24.5 | 13315.603 | 31300.069 | 3193.6600 | 1.117E+00 | 7.000E-19 | 3.650E+05 | 6.94507E+01  | 183 |
| 33.5 | 33.5 | 10571.720 | 31313.400 | 3192.5972 | 6.970E-04 | 3.119E-22 | 1.161E+03 | 6.03073E-01  | 184 |
| 24.5 | 24.5 | 13315.603 | 31313.099 | 3192.5401 | 7.519E-03 | 6.713E-21 | 2.370E+03 | 3.50007E-01  | 185 |
| 34.5 | 34.5 | 10571.720 | 31319.249 | 3191.9990 | 3.250E-02 | 2.047E-26 | 7.390E+04 | 1.30415E+01  | 184 |
| 17.5 | 10.5 | 6122.620  | 31321.421 | 3191.7904 | 3.007E+00 | 1.009E-10 | 2.700E+05 | 1.92064E+01  | 187 |
| 24.5 | 25.5 | 12290.532 | 31326.010 | 3191.3130 | 9.107E-03 | 5.750E-21 | 3.000E+03 | 6.02960E-01  | 184 |
| 25.5 | 25.5 | 12290.532 | 31331.020 | 3190.0025 | 1.101E+00 | 6.903E-19 | 3.640E+05 | 5.13704E+01  | 189 |
| 15.5 | 16.5 | 5525.697  | 31377.379 | 3106.0041 | 3.394E+00 | 2.127E-19 | 2.057E+05 | 1.69662E+01  | 190 |
| 16.5 | 16.5 | 5525.697  | 31300.901 | 3105.7223 | 1.600E-01 | 0.124E-20 | 1.116E+04 | 7.27041E-01  | 191 |
| 23.5 | 23.5 | 10500.267 | 31300.619 | 3103.3327 | 1.663E+00 | 9.169E-19 | 3.090E+05 | 6.74000E+01  | 192 |
| 10.5 | 11.5 | 2944.110  | 31390.949 | 3103.0592 | 1.395E-01 | 0.749E-26 | 7.600E+03 | 2.72600E-01  | 193 |
| 24.5 | 23.5 | 10500.267 | 3143.520  | 3103.5370 | 1.057E-02 | 6.624E-21 | 2.700E+03 | 3.64211E-01  | 194 |
| 10.5 | 11.5 | 5694.652  | 31400.225 | 3102.9500 | 3.504E+00 | 2.240E-10 | 2.020E+05 | 1.02047E+01  | 195 |
| 32.5 | 31.5 | 10513.992 | 31413.067 | 3102.3092 | 5.267E-02 | 3.391E-20 | 9.450E+04 | 1.02047E+01  | 196 |
| 23.5 | 24.5 | 10402.500 | 31416.299 | 3102.1439 | 1.204E-02 | 0.040E-21 | 0.040E+03 | 6.11015E-01  | 197 |
| 24.5 | 24.5 | 10402.500 | 31421.100 | 3101.6657 | 1.052E+00 | 9.100E-19 | 3.690E+05 | 6.93670E+01  | 198 |
| 32.5 | 32.5 | 10593.790 | 31433.969 | 3101.3548 | 7.620E-04 | 9.100E-19 | 1.360E+05 | 6.63617E-01  | 199 |
| 33.5 | 32.5 | 10593.790 | 31439.744 | 3179.7677 | 6.069E-02 | 3.053E-20 | 0.630E+04 | 3.20670E+01  | 200 |

Table 9 (Contd).

| J' J''    | Lower energy vacuum cm <sup>-1</sup> | Transition      | Frequency vacuum cm <sup>-1</sup> | Wavelength SIP angstroms | Intensity cm <sup>-2</sup> atm <sup>-1</sup> | Intensity cm/molecule | Einstein sec <sup>-1</sup> | A Line strength | Number |
|-----------|--------------------------------------|-----------------|-----------------------------------|--------------------------|--|-----------------------|----------------------------|-----------------|--------|
| 39.5 30.5 | 23721.729                            | S R 2 1030.51   | 31453.976                         | 3170.3269                | 1.292E+05                                    | 0.100E+24             | 1.258E+02                  | 1.03093E-01     | 201    |
| 14.5 15.5 | 4932.933                             | P P 2 2015.51   | 31460.396                         | 3177.6003                | 3.953E+00                                    | 2.670E-10             | 2.965E+05                  | 1.59434E+01     | 202    |
| 15.5 15.5 | 4932.933                             | P P 0 1 2015.51 | 31463.010                         | 3177.3355                | 1.022E-01                                    | 1.470E-19             | 1.201E+04                  | 7.67344E-01     | 203    |
| 22.5 22.5 | 9709.502                             | Q Q 2 2022.51   | 31403.056                         | 3175.3124                | 1.009E+00                                    | 1.104E-10             | 6.122E+05                  | 6.54292E-01     | 204    |
| 23.5 22.5 | 9709.602                             | Q Q 1 2022.51   | 31400.600                         | 3174.0332                | 1.673E-02                                    | 9.274E-21             | 3.002E+03                  | 3.74564E-01     | 205    |
| 15.5 16.5 | 4904.629                             | P P 1 1016.51   | 31492.115                         | 3174.4796                | 4.214E+00                                    | 2.71E-10              | 2.442E+05                  | 3.72007E-01     | 206    |
| 9.5 10.5  | 2453.149                             | Q P 1 2010.51   | 31498.667                         | 3173.0193                | 1.734E-01                                    | 1.007E-19             | 9.003E+03                  | 2.90339E-01     | 207    |
| 22.5 23.5 | 9691.321                             | Q Q 2 1023.51   | 31502.136                         | 3172.4697                | 1.774E-02                                    | 1.112E-20             | 3.053E+03                  | 4.21720E-01     | 208    |
| 23.5 23.5 | 9691.321                             | Q Q 0 1 1023.51 | 31506.000                         | 3172.9911                | 1.007E+00                                    | 1.103E-10             | 3.930E+05                  | 4.73570E-01     | 209    |
| 31.5 30.5 | 16652.271                            | R R 2 2030.51   | 31527.110                         | 3170.9550                | 7.640E-02                                    | 4.794E-20             | 1.055E+05                  | 3.02394E-01     | 210    |
| 13.5 14.5 | 4371.265                             | P P 2 2016.51   | 31540.400                         | 3169.6197                | 4.527E+00                                    | 2.037E-10             | 3.007E+05                  | 1.69194E-01     | 211    |
| 14.5 14.5 | 4371.265                             | P P 0 1 2016.51 | 31543.620                         | 3169.2961                | 2.337E-01                                    | 1.465E-19             | 1.470E+04                  | 7.91564E-01     | 212    |
| 31.5 31.5 | 16631.946                            | P Q 2 1031.51   | 31547.443                         | 3160.9120                | 1.157E-03                                    | 7.249E-22             | 1.500E+03                  | 4.49959E-01     | 213    |
| 32.5 31.5 | 16631.946                            | R R 2 1 1031.51 | 31553.160                         | 3160.3371                | 7.156E-02                                    | 4.605E-20             | 9.530E+04                  | 3.10733E-01     | 214    |
| 21.5 21.5 | 8944.563                             | Q Q 2 2021.51   | 31564.701                         | 3167.1793                | 2.410E+00                                    | 1.511E-10             | 4.351E+05                  | 4.34457E-01     | 215    |
| 22.5 21.5 | 8944.563                             | Q Q 1 2021.51   | 31569.309                         | 3166.7171                | 2.035E-02                                    | 1.274E-20             | 3.516E+03                  | 3.06650E-01     | 216    |
| 14.5 15.5 | 4341.046                             | P P 1 1015.51   | 31573.139                         | 3166.3929                | 4.073E+00                                    | 3.054E-10             | 3.059E+05                  | 1.62750E-01     | 217    |
| 21.5 22.5 | 8925.622                             | Q P 2 1022.51   | 31503.642                         | 3165.2799                | 2.429E-02                                    | 1.523E-20             | 4.365E+03                  | 4.57460E-01     | 218    |
| 22.5 22.5 | 8925.622                             | Q Q 1 1022.51   | 31500.250                         | 3164.0102                | 2.410E+00                                    | 1.516E-10             | 4.157E+05                  | 4.57460E-01     | 219    |
| 0.5 9.5   | 2056.560                             | Q P 1 21 9.51   | 31595.731                         | 3164.0607                | 2.137E-01                                    | 1.339E-19             | 1.040E+04                  | 3.10306E-01     | 220    |
| 30.5 37.5 | 22671.446                            | S R 2 1037.51   | 31611.531                         | 3162.4073                | 2.443E-02                                    | 1.531E-20             | 1.027E+02                  | 1.01661E-01     | 221    |
| 12.5 13.5 | 3061.676                             | P P 2 2013.51   | 31617.404                         | 3161.0390                | 5.103E-00                                    | 3.190E-10             | 3.170E+05                  | 1.53917E-01     | 222    |
| 13.5 13.5 | 3061.676                             | P P 0 1 2013.51 | 31620.425                         | 3161.5977                | 2.974E-01                                    | 6.044E-19             | 1.710E+04                  | 8.30293E-01     | 223    |
| 30.5 29.5 | 1709.237                             | R R 2 2020.51   | 31633.567                         | 3160.2062                | 1.096E-01                                    | 6.047E-20             | 1.170E+05                  | 2.92407E-01     | 224    |
| 20.5 20.5 | 8206.027                             | Q Q 2 2020.51   | 31641.266                         | 3159.5152                | 3.031E+00                                    | 1.900E-10             | 4.572E+05                  | 4.1002E-01      | 225    |
| 21.5 20.5 | 8206.027                             | Q R 1 2020.51   | 31645.722                         | 3159.0702                | 2.779E-02                                    | 1.742E-20             | 4.003E+03                  | 3.90021E-01     | 226    |
| 13.5 14.5 | 3010.759                             | P P 1 1014.51   | 31651.343                         | 3150.5052                | 5.540E+00                                    | 3.472E-10             | 3.172E+05                  | 1.57695E-01     | 227    |
| 30.5 30.5 | 15600.670                            | R R 2 1030.51   | 31656.113                         | 3150.2320                | 1.729E-03                                    | 1.004E-21             | 1.037E+03                  | 4.50553E-01     | 228    |
| 31.5 30.5 | 15600.670                            | R R 1 1030.51   | 31659.760                         | 3157.6695                | 1.033E-01                                    | 6.474E-20             | 1.063E+05                  | 3.00700E-01     | 229    |
| 20.5 21.5 | 8106.350                             | Q Q 2 1021.51   | 31660.935                         | 3157.5523                | 3.291E-02                                    | 2.003E-20             | 4.940E+03                  | 4.45149E-01     | 230    |
| 21.5 21.5 | 8106.350                             | Q Q 0 1 1021.51 | 31665.391                         | 3157.1000                | 3.059E+00                                    | 1.917E-10             | 6.304E+05                  | 4.33330E-01     | 231    |
| 7.5 0.5   | 1694.914                             | Q P 1 21 0.51   | 31600.020                         | 3154.6534                | 2.609E-01                                    | 1.635E-19             | 3.267E+05                  | 1.26593E-01     | 232    |
| 11.5 12.5 | 3344.522                             | P P 2 2012.51   | 31691.411                         | 3154.5157                | 5.645E+00                                    | 3.300E-10             | 2.005E+04                  | 1.82070E-01     | 233    |
| 19.5 19.5 | 7494.040                             | Q Q 2 2019.51   | 31713.653                         | 3152.3033                | 3.750E+00                                    | 2.335E-10             | 6.704E+05                  | 3.93025E-01     | 234    |
| 20.5 19.5 | 7494.040                             | Q Q 1 2019.51   | 31694.220                         | 3154.2353                | 3.752E-01                                    | 2.352E-19             | 2.005E+04                  | 1.82070E-01     | 235    |
| 22.5 13.5 | 3311.902                             | Q P 1 1013.51   | 31717.653                         | 3152.3033                | 3.750E+00                                    | 2.335E-10             | 6.704E+05                  | 3.93025E-01     | 236    |
| 12.5 12.5 | 3344.522                             | P P 0 2 2012.51 | 31691.411                         | 3154.5157                | 5.645E+00                                    | 3.300E-10             | 2.005E+04                  | 1.82070E-01     | 237    |
| 29.5 20.5 | 14705.263                            | R R 2 2020.51   | 31736.423                         | 3150.3472                | 1.541E-01                                    | 9.601E-20             | 1.202E+05                  | 4.567E+03       | 238    |
| 19.5 20.5 | 7474.376                             | Q P 2 1020.51   | 31734.125                         | 3150.2696                | 4.422E-02                                    | 2.391E-10             | 9.604E+03                  | 4.50959E-01     | 239    |
| 20.5 20.5 | 7474.376                             | Q Q 1 1020.51   | 31730.423                         | 3149.0430                | 3.015E+00                                    | 2.391E-10             | 6.604E+05                  | 4.13107E-01     | 240    |
| 29.5 29.5 | 14764.034                            | P Q 2 1029.51   | 31754.173                         | 3140.2006                | 2.554E-03                                    | 1.600E-21             | 2.112E+03                  | 4.50970E-01     | 241    |
| 37.5 36.5 | 21633.610                            | S R 2 1036.51   | 31759.597                         | 3147.7429                | 4.274E-05                                    | 2.675E-23             | 1.394E+02                  | 1.00437E-01     | 242    |
| 30.5 29.5 | 14764.034                            | R R 1 1029.51   | 31750.733                         | 3147.7294                | 1.470E-01                                    | 9.215E-20             | 1.172E+05                  | 2.90020E-01     | 243    |
| 10.5 11.5 | 2800.525                             | P P 2 2011.51   | 31762.412                         | 3147.4619                | 6.127E+00                                    | 3.046E-20             | 3.362E+05                  | 1.10217E-01     | 244    |
| 11.5 11.5 | 2800.525                             | P P 0 1 2011.51 | 31765.021                         | 3147.2054                | 4.690E-01                                    | 2.940E-19             | 2.350E+04                  | 9.24097E-01     | 245    |
| 6.5 7.5   | 1368.720                             | Q P 1 21 7.51   | 31701.413                         | 3145.5921                | 3.151E-01                                    | 1.955E-19             | 1.690E+04                  | 3.57791E-01     | 246    |
| 12.5 10.5 | 6011.055                             | Q Q 2 2010.51   | 31701.956                         | 3145.5204                | 4.505E+00                                    | 2.674E-10             | 4.900E+05                  | 3.73022E-01     | 247    |

|      |      |           |   |   |   |         |           |            |           |           |             |             |     |
|------|------|-----------|---|---|---|---------|-----------|------------|-----------|-----------|-------------|-------------|-----|
| 19.5 | 10.5 | 6011.055  | 0 | R | 1 | 2110.51 | 31706.009 | 5.849E-02  | 3.164E-20 | 5.217E+03 | 4.20701E-01 | 240         |     |
| 11.5 | 12.5 | 2064.009  | 0 | P | 1 | 1112.51 | 31799.556 | 6.022E+00  | 9.276E-10 | 3.402E+05 | 1.32510E+01 | 249         |     |
| 10.5 | 19.5 | 6790.493  | 0 | 0 | 2 | 1119.51 | 31803.310 | 5.905E-62  | 3.691E-20 | 6.370E+03 | 0.74397E-01 | 248         |     |
| 19.5 | 19.5 | 6790.693  | 0 | 0 | 1 | 1119.51 | 31807.452 | 4.600E+00  | 2.930E-19 | 4.019E+05 | 3.93012E+01 | 251         |     |
| 20.5 | 27.5 | 13901.320 | 0 | R | 2 | 2127.51 | 31826.709 | 2.143E-01  | 1.343E-19 | 1.390E+05 | 2.72512E+01 | 252         |     |
| 9.5  | 10.5 | 2450.279  | 0 | P | 0 | 2110.51 | 31830.303 | 6.510E+05  | 3.00E-10  | 3.440E+05 | 1.07700E+01 | 253         |     |
| 10.5 | 16.5 | 2450.279  | 0 | 0 | 1 | 2110.51 | 31832.700 | 5.016E-61  | 3.646E-19 | 2.081E+04 | 9.00044E-01 | 254         |     |
| 17.5 | 17.5 | 6157.054  | 0 | 0 | 2 | 2117.51 | 31846.260 | 5.520E+00  | 3.400E-10 | 5.109E+05 | 3.53391E+01 | 255         |     |
| 20.5 | 20.5 | 13060.205 | 0 | R | 0 | 2120.51 | 31857.024 | 3.139.1767 | 2.336E-21 | 2.810E+03 | 4.66291E+01 | 256         |     |
| 10.5 | 17.5 | 6157.054  | 0 | P | 1 | 2117.51 | 31853.222 | 6.700E-02  | 4.204E-20 | 5.971E+03 | 4.66359E-01 | 257         |     |
| 29.5 | 20.5 | 13060.205 | 0 | R | 1 | 1120.51 | 31853.291 | 2.055E-01  | 1.200E-19 | 1.200E+07 | 2.00050F+01 | 258         |     |
| 17.5 | 10.5 | 6135.500  | 0 | 0 | 2 | 1110.51 | 31869.613 | 7.769E-02  | 4.070E-20 | 7.250E+03 | 4.91600E-01 | 259         |     |
| 10.5 | 11.5 | 2413.613  | 0 | P | 1 | 1111.51 | 31869.666 | 3.316E+05  | 6.817E-10 | 3.516E+05 | 1.22402E+01 | 260         |     |
| 5.5  | 6.5  | 1070.509  | 0 | 0 | 1 | 21      | 31869.725 | 3.752E-01  | 2.102E+04 | 2.102E+04 | 3.06410E-01 | 261         |     |
| 10.5 | 10.5 | 6135.500  | 0 | 0 | 1 | 1110.51 | 31872.576 | 5.569E+00  | 3.553E-10 | 5.010E+05 | 3.72011E+01 | 262         |     |
| 0.5  | 9.5  | 2056.353  | 0 | P | 2 | 21      | 31895.203 | 6.766E+00  | 6.240E-10 | 3.532E+05 | 9.72727E+00 | 263         |     |
| 9.5  | 9.5  | 2056.353  | 0 | 0 | 1 | 21      | 31897.563 | 7.146E-01  | 4.479E-19 | 3.359E+04 | 1.04530E+00 | 264         |     |
| 36.5 | 35.5 | 20600.506 | 0 | S | 0 | 2135.51 | 31898.447 | 7.124E-05  | 4.465E-23 | 3.000E+02 | 1.79406E-01 | 265         |     |
| 16.5 | 16.5 | 5533.620  | 0 | 0 | 2 | 2116.51 | 31966.642 | 6.546E+00  | 4.102E-10 | 5.379E+05 | 3.33129E+01 | 266         |     |
| 27.5 | 26.5 | 12990.371 | 0 | R | 2 | 2126.51 | 31913.035 | 2.930E-01  | 5.939E-20 | 6.051E+03 | 4.65976E-01 | 267         |     |
| 16.5 | 17.5 | 5510.159  | 0 | 0 | 2 | 1117.51 | 31930.104 | 1.019E-01  | 6.300E-20 | 0.209E+03 | 5.11063E-01 | 269         |     |
| 17.5 | 17.5 | 5510.159  | 0 | 0 | 1 | 1117.51 | 31933.009 | 6.730E+00  | 4.230E-10 | 5.210E+05 | 3.52579E+01 | 270         |     |
| 27.5 | 27.5 | 12976.943 | 0 | 0 | 2 | 1127.51 | 31935.264 | 5.306E-03  | 3.374E-21 | 2.759E+03 | 3.62506E-01 | 271         |     |
| 9.5  | 10.5 | 2015.036  | 0 | P | 1 | 1110.51 | 31936.741 | 7.790E+00  | 4.006E-10 | 3.620E+05 | 1.12265E+01 | 272         |     |
| 20.5 | 27.5 | 12976.943 | 0 | R | 1 | 1127.51 | 31943.630 | 2.036E-01  | 1.770E-19 | 1.406E+05 | 2.70072E+01 | 273         |     |
| 4.5  | 5.5  | 026.013   | 0 | 0 | 1 | 21      | 31954.665 | 4.309E-01  | 2.751E-19 | 2.019E+04 | 4.10930E-01 | 274         |     |
| 7.5  | 8.5  | 1693.290  | 0 | 0 | 2 | 21      | 31957.049 | 6.058E+00  | 4.297E-10 | 3.611E+05 | 0.66026E+00 | 275         |     |
| 0.5  | 0.5  | 1693.290  | 0 | 0 | 1 | 21      | 31959.000 | 0.707E-01  | 5.450E-19 | 4.077E+04 | 1.11050E+00 | 276         |     |
| 15.5 | 15.5 | 4939.902  | 0 | 0 | 2 | 2115.51 | 31963.173 | 7.629E+00  | 4.702E-10 | 5.549E+05 | 3.12030E+01 | 277         |     |
| 16.5 | 15.5 | 4939.902  | 0 | 0 | 1 | 2115.51 | 31966.776 | 1.150E-01  | 7.213E-20 | 7.077E+01 | 4.17917E-01 | 278         |     |
| 15.5 | 16.5 | 4915.197  | 0 | 0 | 2 | 1116.51 | 31907.077 | 1.319E-01  | 0.245E-20 | 9.500E+03 | 5.32052E-01 | 279         |     |
| 16.5 | 16.5 | 4915.197  | 0 | 0 | 1 | 1116.51 | 31991.600 | 7.943E+00  | 4.970E-10 | 5.605E+05 | 3.32314E+01 | 280         |     |
| 26.5 | 25.5 | 12137.370 | 0 | R | 2 | 2125.51 | 31994.965 | 3.966E-01  | 2.409E-19 | 1.627E+05 | 2.52636E+01 | 281         |     |
| 0.5  | 9.5  | 1659.790  | 0 | P | 1 | 11      | 32061.509 | 0.003E+00  | 5.066E-10 | 3.745E+05 | 1.02106E+01 | 282         |     |
| 6.5  | 7.5  | 1367.617  | 0 | P | 2 | 21      | 32015.547 | 6.746E+00  | 4.227E-10 | 3.500E+05 | 7.59906E+00 | 283         |     |
| 16.5 | 16.5 | 4377.619  | 0 | 0 | 2 | 2114.51 | 32015.910 | 0.750E+00  | 5.404E-10 | 5.713E+05 | 2.92491E+01 | 284         |     |
| 26.5 | 26.5 | 12115.590 | 0 | 0 | 2 | 1126.51 | 32016.677 | 7.602E-03  | 4.015E-21 | 3.134E+03 | 4.01406E-01 | 285         |     |
| 7.5  | 7.5  | 1367.617  | 0 | P | 1 | 21      | 32017.324 | 1.051E+00  | 6.590E-10 | 5.020E+04 | 1.20092E+00 | 286         |     |
| 15.5 | 14.5 | 4377.619  | 0 | 0 | R | 1       | 2114.51   | 32019.325  | 1.407E-01 | 9.322E-20 | 9.405E+03   | 5.12512E-01 | 287 |
| 27.5 | 26.5 | 12115.590 | 0 | R | 1 | 1126.51 | 32021.935 | 3.460E-01  | 2.426E-19 | 1.519E+05 | 2.60003E+01 | 288         |     |
| 35.5 | 34.5 | 19597.902 | 0 | S | 0 | 2134.51 | 32024.345 | 1.136E-04  | 7.123E-23 | 3.516E+02 | 1.70756E-01 | 289         |     |
| 3.5  | 4.5  | 600.194   | 0 | 0 | 1 | 21      | 32035.976 | 4.996E-01  | 3.131E-19 | 3.676E+04 | 4.32924E-01 | 290         |     |
| 14.5 | 15.5 | 4351.310  | 0 | 0 | 2 | 1115.51 | 32042.019 | 1.609E-01  | 1.050E-19 | 1.095E+04 | 5.57613E-01 | 291         |     |
| 15.5 | 15.5 | 4351.310  | 0 | 0 | 1 | 1115.51 | 32045.423 | 9.171E+05  | 5.740E-10 | 5.577E+05 | 3.12011E+01 | 292         |     |
| 7.5  | 0.5  | 1321.252  | 0 | P | 1 | 11      | 32063.690 | 0.195E+00  | 5.136E-10 | 3.060E+05 | 9.12055E+00 | 293         |     |
| 13.5 | 13.5 | 3046.059  | 0 | 0 | 2 | 2113.51 | 32064.966 | 9.066E+00  | 6.104E-10 | 5.066E+05 | 2.72100E+01 | 294         |     |
| 14.5 | 13.5 | 3046.059  | 0 | 0 | 1 | 2113.51 | 32069.126 | 1.945E-01  | 1.193E-19 | 1.763E+04 | 5.40150E-01 | 295         |     |
| 25.5 | 24.5 | 11299.250 | 0 | R | 2 | 2124.51 | 32070.095 | 5.204E-01  | 3.317E-19 | 1.743E+05 | 2.62675E+01 | 296         |     |
| 5.5  | 6.5  | 1077.054  | 0 | P | 2 | 21      | 32070.760 | 6.405E+00  | 4.010E-10 | 3.737E+05 | 6.52103E+00 | 297         |     |
| 6.5  | 6.5  | 1077.054  | 0 | 0 | 1 | 21      | 32072.279 | 1.255E+00  | 7.045E-19 | 6.276E+04 | 1.29194E+00 | 298         |     |
| 25.5 | 25.5 | 11277.107 | 0 | P | 2 | 1125.51 | 32092.245 | 1.006E-02  | 6.009E-21 | 3.556E+03 | 4.91267E-01 | 299         |     |
| 13.5 | 14.5 | 3019.156  | 0 | 0 | 2 | 1114.51 | 32092.600 | 2.147E-01  | 1.346E-19 | 1.267E+04 | 5.05109E-01 | 300         |     |

Table 9 (Contd.)

| J' J''    | Lower energy vacuum cm <sup>-1</sup> | Transition    | Frequency vacuum cm <sup>-1</sup> | Wavelength STP angstroms | Intensity cm <sup>-2</sup> atm <sup>-1</sup> | Intensity cm/molecule | Einstein A sec <sup>-1</sup> | Line strength | Number |
|-----------|--------------------------------------|---------------|-----------------------------------|--------------------------|--|-----------------------|------------------------------|---------------|--------|
| 14.5 14.5 | 3019.156 -                           | Q 1 1114.51   | 32095.029                         | 3114.7633                | 1.042E+01                                    | 6.520E-10             | 5.739E+05                    | 2.91645E+01   | 301    |
| 26.5 25.5 | 13277.107 -                          | R R 1 1425.51 | 32097.380                         | 3114.6158                | 5.170E-51                                    | 3.245E-19             | 1.631E+05                    | 2.50004E+01   | 302    |
| 12.5 12.5 | 3360.000 +                           | Q 2 2112.51   | 32110.200                         | 3113.3722                | 1.033E+01                                    | 6.050E-10             | 6.002E+05                    | 2.51660E+01   | 303    |
| 2.5 3.5   | 629.272 -                            | Q P 1 21 3.51 | 32113.213                         | 3113.0081                | 5.417E-01                                    | 3.399E-19             | 5.175E+04                    | 6.60599E-01   | 304    |
| 13.5 12.5 | 3160.000 +                           | Q R 1 2112.51 | 32113.222                         | 3113.0792                | 2.416E-01                                    | 1.514E-19             | 1.232E+04                    | 5.71279E-01   | 305    |
| 6.5 5.5   | 824.525 +                            | P P 2 21 5.51 | 32122.605                         | 3112.1022                | 5.032E+00                                    | 3.656E-10             | 3.705E+05                    | 5.43172E+00   | 306    |
| 6.5 7.5   | 1026.730 -                           | P P 1 11 7.51 | 32123.403                         | 3112.0925                | 0.095E+00                                    | 5.074E-10             | 3.597E+05                    | 0.17260E+00   | 307    |
| 5.5 5.5   | 824.525 +                            | P Q 1 21 5.51 | 32123.609                         | 3112.0658                | 1.478E+00                                    | 9.261E-19             | 7.591E+04                    | 1.30079E+00   | 308    |
| 24.5 23.5 | 10404.962 +                          | R R 2 2123.51 | 32139.570                         | 3110.5270                | 6.946E-61                                    | 4.354E-19             | 1.052E+05                    | 2.32710E+01   | 309    |
| 12.5 13.5 | 3319.355 +                           | Q P 2 1113.51 | 32139.725                         | 3110.5120                | 2.711E-01                                    | 1.700E-19             | 1.670E+04                    | 6.16716E-01   | 310    |
| 13.5 13.5 | 3319.355 +                           | Q Q 1 1113.51 | 32142.747                         | 3110.2196                | 1.163E+61                                    | 7.209E-10             | 5.000E+05                    | 2.71260E+01   | 311    |
| 16.5 33.5 | 1862.331 +                           | S R 2 1133.51 | 32149.545                         | 3109.5610                | 1.706E-04                                    | 1.119E-22             | 4.311E+02                    | 1.70260E-01   | 312    |
| 11.5 11.5 | 2004.110 -                           | Q Q 2 2111.51 | 32151.022                         | 3109.3416                | 1.106E+01                                    | 7.435E-10             | 6.120E+05                    | 2.31170E+01   | 313    |
| 12.5 11.5 | 2004.110 -                           | Q R 1 2111.51 | 32154.640                         | 3109.0651                | 3.039E-01                                    | 1.905E-19             | 1.647E+04                    | 6.06410E-01   | 314    |
| 24.5 24.5 | 10402.394 +                          | R R 2 2124.51 | 32162.139                         | 3108.3462                | 1.520E-02                                    | 9.530E-21             | 4.031E+03                    | 5.01057E-01   | 315    |
| 25.5 24.5 | 10402.394 +                          | R R 1 1124.51 | 32167.150                         | 3107.0591                | 6.046E-01                                    | 4.291E-19             | 1.746E+05                    | 2.40074E-01   | 316    |
| 3.5 4.5   | 600.100 -                            | P P 2 21 4.51 | 32170.237                         | 3107.5617                | 5.022E+00                                    | 3.140E-10             | 3.019E+05                    | 4.33399E+00   | 317    |
| 4.5 4.5   | 600.100 -                            | P Q 1 21 4.51 | 32171.290                         | 3107.6600                | 1.795E+00                                    | 1.069E-10             | 1.037E+05                    | 1.40361E+00   | 318    |
| 5.5 4.5   | 767.450 +                            | P P 1 11 6.51 | 32180.756                         | 3106.5459                | 7.748E+00                                    | 4.069E-10             | 6.141E+05                    | 7.15200E+00   | 319    |
| 11.5 12.5 | 2052.405 -                           | Q P 2 1112.51 | 32183.640                         | 3106.2066                | 3.333E-01                                    | 2.127E-19             | 1.737E+04                    | 6.52643E-01   | 320    |
| 1.5 2.5   | 200.769 +                            | Q Q 1 21 2.51 | 32185.069                         | 3106.0592                | 5.316E-01                                    | 3.340E-19             | 7.357E+04                    | 4.15554E-01   | 321    |
| 12.5 12.5 | 2052.405 -                           | Q Q 1 1112.51 | 32186.266                         | 3106.0151                | 1.275E+01                                    | 7.992E-10             | 6.025E+05                    | 2.50015E+01   | 322    |
| 10.5 10.5 | 2653.149 +                           | Q Q 2 2110.51 | 32189.707                         | 3105.6733                | 1.282E+01                                    | 7.900E-10             | 6.220E+05                    | 2.10604E+01   | 323    |
| 11.5 16.5 | 2653.149 +                           | Q R 1 2110.51 | 32192.397                         | 3105.4225                | 3.706E-01                                    | 3.700E-19             | 1.711E+04                    | 6.46105E-01   | 324    |
| 23.5 22.5 | 9695.394 -                           | R R 2 2122.51 | 32203.691                         | 3104.3526                | 9.600E-01                                    | 5.641E-19             | 1.961E+04                    | 2.22737E+01   | 325    |
| 2.5 3.5   | 429.450 +                            | P P 2 21 3.51 | 32213.092                         | 3103.3593                | 3.990E+00                                    | 2.501E-10             | 3.035E+05                    | 3.23470E+00   | 326    |
| 3.5 3.5   | 429.450 +                            | P Q 1 21 3.51 | 32214.713                         | 3103.2712                | 1.910E+00                                    | 1.197E-10             | 1.377E+05                    | 1.55030E+00   | 327    |
| 10.5 11.5 | 2419.001 +                           | Q P 2 1111.51 | 32223.055                         | 3102.3908                | 6.215E-61                                    | 2.642E-19             | 2.060E+04                    | 6.93759E-01   | 328    |
| 9.5 9.5   | 2056.560 -                           | Q Q 2 21 9.51 | 32226.095                         | 3102.3677                | 1.311E+01                                    | 0.217E-10             | 6.259E+05                    | 1.09962E+01   | 329    |
| 11.5 11.5 | 2419.001 +                           | Q Q 1 1111.51 | 32226.466                         | 3102.1396                | 1.378E+61                                    | 0.507E-10             | 6.139E+05                    | 2.30295E+01   | 330    |
| 10.5 9.5  | 2056.560 -                           | Q R 1 21 9.51 | 32226.492                         | 3102.1369                | 4.676E-01                                    | 2.931E-19             | 6.041E+04                    | 6.90930E-01   | 331    |
| 23.5 23.5 | 9672.362 -                           | P Q 2 1123.51 | 32226.524                         | 3102.1334                | 2.107E-02                                    | 1.320E-20             | 4.536E+03                    | 5.13700E-01   | 332    |
| 24.5 23.5 | 9672.362 -                           | R R 1 1123.51 | 32231.413                         | 3101.6632                | 0.910E-01                                    | 5.505E-19             | 1.053E+05                    | 2.13050E+01   | 333    |
| 4.5 5.5   | 563.575 -                            | P P 1 11 5.51 | 32235.003                         | 3101.2312                | 7.216E+00                                    | 4.523E-10             | 6.310E+05                    | 6.13324E+00   | 334    |
| 1.5 2.5   | 209.041 -                            | P P 2 21 2.51 | 32252.060                         | 3099.6807                | 2.702E+03                                    | 1.744E-10             | 3.040E+05                    | 2.14901E+00   | 335    |
| 5.5 1.5   | 107.491 -                            | Q P 1 21 1.51 | 32253.649                         | 3099.5025                | 4.156E-01                                    | 2.605E-19             | 1.114E+05                    | 3.1012E-01    | 336    |
| 2.5 2.5   | 209.041 -                            | P Q 1 21 2.51 | 32253.647                         | 3099.5453                | 2.033E+00                                    | 1.274E-10             | 1.075E+05                    | 1.57754E+00   | 337    |
| 0.5 0.5   | 1694.914 +                           | Q Q 2 21 0.51 | 32254.722                         | 3099.4217                | 1.329E+61                                    | 0.329E-10             | 6.142E+05                    | 1.69230E+01   | 338    |
| 9.5 0.5   | 1694.914 +                           | Q Q 1 21 0.51 | 32256.902                         | 3099.2122                | 5.723E-01                                    | 3.507E-19             | 2.450E+04                    | 7.41400E-01   | 339    |
| 9.5 10.5  | 2019.633 +                           | Q P 2 1110.51 | 32261.029                         | 3098.0150                | 5.191E+00                                    | 3.253E-19             | 2.446E+04                    | 7.61015E-01   | 340    |
| 22.5 21.5 | 0931.646 +                           | R R 2 2121.51 | 32262.011                         | 3098.7255                | 1.151E+00                                    | 7.215E-22             | 5.060E+05                    | 2.12757E+01   | 341    |
| 33.5 32.5 | 17622.044 -                          | S R 2 1132.51 | 32262.292                         | 3098.6995                | 2.740E-04                                    | 1.072E-22             | 5.063E+02                    | 1.70036E-01   | 342    |
| 10.5 16.5 | 2019.633 +                           | Q Q 1 1110.51 | 32263.426                         | 3098.5056                | 1.442E+01                                    | 9.000E-10             | 6.236E+05                    | 2.09700E+01   | 343    |
| 7.5 7.5   | 1360.720 -                           | Q Q 2 21 7.51 | 32201.619                         | 3096.5032                | 1.310E+01                                    | 0.209E-10             | 6.356E+05                    | 1.60431E+01   | 344    |
| 0.5 7.5   | 1360.720 -                           | Q R 1 21 7.51 | 32203.579                         | 3096.6512                | 6.920E-01                                    | 4.342E-19             | 2.591E+04                    | 7.97604E-01   | 345    |
| 22.5 22.5 | 8907.090 +                           | P Q 2 1122.51 | 32205.559                         | 3096.4612                | 2.009E-02                                    | 1.011E-20             | 5.160E+03                    | 5.27171E-01   | 346    |
| .5 1.5    | 107.751 +                            | P P 2 21 1.51 | 32206.475                         | 3096.3734                | 1.478E+00                                    | 9.264E-19             | 3.970E+05                    | 1.10190E+00   | 347    |





Table 9 (Contd).

| J' J''    | Lower energy vacuum cm <sup>-1</sup> | Transition      | Frequency vacuum cm <sup>-1</sup> | Wavelength SIP angstroms | Intensity cm <sup>-2</sup> atm <sup>-1</sup> | Intensity cm/molecule | Einstein sec <sup>-1</sup> | A Line strength | Number |
|-----------|--------------------------------------|-----------------|-----------------------------------|--------------------------|--|-----------------------|----------------------------|-----------------|--------|
| 1.5 1.5   | .056 *                               | Q 0 1 1c 1.5i   | 32476.523                         | 3070.4520                | 3.207E+00                                    | 2.00E-10              | 6.30E+05                   | 2.24021E+00     | 401    |
| 1.5 1.5   | 6122.620 *                           | R R 1 1010.5i   | 32475.317                         | 3070.3675                | 3.694E+00                                    | 1.60E-10              | 5.36E+05                   | 1.0500E+01      | 402    |
| 1.5 1.5   | 5225.697 -                           | R R 2 2016.5i   | 32470.617                         | 3070.6737                | 3.146E+00                                    | 1.97E-10              | 2.52E+05                   | 1.6272E+01      | 403    |
| 3.5 2.5   | 209.061 -                            | R R 2 2i 2.5i   | 32409.304                         | 3077.0346                | 2.933E+00                                    | 1.03E-10              | 2.05E+05                   | 2.2727E+00      | 404    |
| 17.5 17.5 | 5490.452 -                           | R R 2 1017.5i   | 32505.661                         | 3075.4937                | 1.219E-01                                    | 7.64E-20              | 9.70E+03                   | 6.22121E-01     | 405    |
| 16.5 15.5 | 4932.933 *                           | R R 2 2015.5i   | 32507.330                         | 3075.3350                | 3.669E+00                                    | 2.30E-10              | 2.59E+05                   | 1.5200E+01      | 406    |
| 16.5 17.5 | 5490.452 -                           | R R 1 1017.5i   | 32509.624                         | 3075.1100                | 3.212E+00                                    | 2.01E-10              | 2.42E+05                   | 1.70304E+01     | 407    |
| 6.5 3.5   | 629.450 *                            | R R 2 2i 3.5i   | 32517.473                         | 3074.3765                | 3.936E+00                                    | 2.46E-10              | 2.31E+05                   | 3.20653E+00     | 408    |
| 15.5 16.5 | 4371.365 -                           | R R 2 2016.5i   | 32531.710                         | 3073.0310                | 4.214E+00                                    | 2.64E-10              | 2.65E+05                   | 1.6537E+01      | 409    |
| 16.5 16.5 | 4904.629 *                           | R R 2 1016.5i   | 32535.634                         | 3072.6483                | 1.501E-01                                    | 9.91E-20              | 1.10E+04                   | 6.40424E-01     | 410    |
| 17.5 16.5 | 4904.629 *                           | R R 1 1016.5i   | 32530.420                         | 3072.3020                | 3.770E+00                                    | 2.36E-10              | 2.49E+05                   | 1.60236E+01     | 411    |
| 5.5 4.5   | 600.100 -                            | R R 2 2i 4.5i   | 32540.433                         | 3072.2072                | 4.017E+00                                    | 3.01E-10              | 2.69E+05                   | 1.1037E+00      | 412    |
| 1.5 1.5   | 0.000 -                              | R R 2 1c 1.5i   | 32541.941                         | 3072.0586                | 1.402E+00                                    | 0.70E-19              | 1.00E+05                   | 9.0002E-01      | 413    |
| 2.5 1.5   | 0.000 -                              | R R 1 1i 1.5i   | 32562.404                         | 3072.0131                | 9.434E-01                                    | 5.91E-19              | 0.091E+04                  | 6.62669E-01     | 414    |
| 16.5 15.5 | 3041.676 *                           | R R 2 2013.5i   | 32551.652                         | 3071.1403                | 4.751E+00                                    | 2.97E-10              | 2.71E+05                   | 1.3257E+01      | 415    |
| 16.5 20.5 | 14790.657 *                          | S R 2 1020.5i   | 32552.137                         | 3071.1025                | 9.197E-04                                    | 5.76E-22              | 7.06E+02                   | 1.70954E-01     | 416    |
| 6.5 5.5   | 024.525 *                            | R R 2 2i 5.5i   | 32550.679                         | 3070.4955                | 5.521E+00                                    | 3.46E-10              | 2.62E+05                   | 5.17021E+00     | 417    |
| 2.5 2.5   | 03.719 *                             | R R 0 2 1c 2.5i | 32559.631                         | 3070.3956                | 1.766E+00                                    | 1.10E-10              | 1.55E+05                   | 1.27305E+00     | 418    |
| 3.5 2.5   | 03.719 *                             | R R 1 1c 2.5i   | 32560.452                         | 3070.3102                | 2.124E+00                                    | 1.33E-10              | 1.404E+05                  | 1.5400E+00      | 419    |
| 15.5 15.5 | 4341.046 -                           | R R 2 1015.5i   | 32561.229                         | 3070.2450                | 2.031E-01                                    | 1.27E-19              | 1.271E+04                  | 6.77930E-01     | 420    |
| 16.5 15.5 | 4341.046 -                           | R R 1 1015.5i   | 32564.051                         | 3069.9053                | 4.346E+02                                    | 3.72E-10              | 2.561E+05                  | 1.50062E+01     | 421    |
| 13.5 12.5 | 3344.522 -                           | R R 2 2012.5i   | 32567.242                         | 3069.6700                | 5.261E+00                                    | 3.29E-10              | 2.75E+05                   | 1.2250E+01      | 422    |
| 7.5 6.5   | 1077.054 -                           | R R 2 2i 6.5i   | 32572.405                         | 3069.1044                | 6.014E+00                                    | 7.77E-10              | 2.73E+05                   | 6.10407E+00     | 423    |
| 3.5 3.5   | 201.922 -                            | R R 0 2 1c 3.5i | 32576.504                         | 3068.0053                | 1.709E+00                                    | 1.12E-10              | 1.22E+05                   | 1.34301E+00     | 424    |
| 4.5 3.5   | 201.922 -                            | R R 1 1i 3.5i   | 32577.557                         | 3068.7061                | 3.334E+00                                    | 2.09E-10              | 1.031E+05                  | 2.52505E+00     | 425    |
| 12.5 11.5 | 2000.525 *                           | R R 2 2011.5i   | 32570.555                         | 3068.6120                | 5.714E+00                                    | 3.50E-10              | 2.791E+05                  | 1.24516E+01     | 426    |
| 8.5 7.5   | 1367.617 *                           | R R 2 2i 7.5i   | 32502.019                         | 3060.2959                | 6.310E+00                                    | 3.95E-10              | 2.77E+05                   | 7.11950E+00     | 427    |
| 14.5 14.5 | 3010.759 *                           | R R 0 2 1114.5i | 32502.570                         | 3060.2339                | 2.505E-01                                    | 1.62E-19              | 1.464E+04                  | 7.11106E-01     | 428    |
| 11.5 10.5 | 2500.279 *                           | R R 2 1014.5i   | 32505.953                         | 3067.9436                | 6.074E+00                                    | 3.00E-10              | 2.61E+05                   | 1.02315E+01     | 429    |
| 15.5 15.5 | 3010.759 *                           | R R 1 1014.5i   | 32505.605                         | 3067.9124                | 6.932E+00                                    | 3.09E-10              | 2.61E+05                   | 1.30660E+01     | 430    |
| 9.5 8.5   | 1093.290 -                           | R R 2 2i 8.5i   | 32507.372                         | 3067.7010                | 6.404E+00                                    | 4.01E-10              | 2.00E+05                   | 6.20015E+00     | 431    |
| 10.5 9.5  | 2054.353 *                           | R R 2 2c 9.5i   | 32500.503                         | 3067.6670                | 6.315E+00                                    | 3.95E-10              | 2.01E+05                   | 9.22020E+00     | 432    |
| 6.5 4.5   | 395.105 *                            | R R 0 2 1c 4.5i | 32591.026                         | 3067.3626                | 1.660E+00                                    | 1.04E-10              | 0.577E+04                  | 1.2173E+00      | 433    |
| 5.5 4.5   | 355.105 *                            | R R 1 1c 4.5i   | 32593.109                         | 3067.2510                | 4.445E+00                                    | 2.17E+05              | 2.33E+05                   | 3.55940E+00     | 434    |
| 13.5 13.5 | 3311.902 -                           | R R 0 2 1013.5i | 32599.703                         | 3066.6310                | 3.262E-01                                    | 2.04E-19              | 1.695E+04                  | 7.40441E-01     | 435    |
| 14.5 13.5 | 3311.902 -                           | R R 1 1013.5i   | 32603.003                         | 3066.3109                | 5.491E+00                                    | 3.44E-10              | 2.664E+05                  | 1.29624E+01     | 436    |
| 5.5 5.5   | 543.575 -                            | R R 0 2 1i 5.5i | 32605.046                         | 3066.1100                | 1.475E+00                                    | 9.24E-19              | 7.52E+04                   | 1.25109E+01     | 437    |
| 6.5 5.5   | 543.575 -                            | R R 1 1i 5.5i   | 32606.557                         | 3065.9766                | 5.370E+00                                    | 3.37E-10              | 2.35E+05                   | 4.61326E+00     | 438    |
| 12.5 12.5 | 2046.009 *                           | R R 0 2 1012.5i | 32612.991                         | 3065.3710                | 4.000E-01                                    | 2.55E-19              | 1.975E+04                  | 7.90527E-01     | 439    |

|      |      |           |   |   |   |         |           |           |           |           |           |           |             |     |
|------|------|-----------|---|---|---|---------|-----------|-----------|-----------|-----------|-----------|-----------|-------------|-----|
| 6.5  | 6.5  | 767.458   | R | 7 | 2 | 11      | 6.51      | 32615.746 | 3055.1124 | 1.276E+00 | 7.997E-19 | 5.909E+04 | 1.17227E+00 | 440 |
| 13.5 | 12.5 | 2046.009  | R | R | 1 | 1012.51 | 32616.012 | 3065.0079 | 5.999E+00 | 5.999E+00 | 3.760E-10 | 2.697E+05 | 1.19353E+01 | 441 |
| 7.5  | 6.5  | 767.458   | R | R | 1 | 10.51   | 32617.404 | 3066.9496 | 6.090E+00 | 6.090E+00 | 3.017E-10 | 2.507E+05 | 5.67107E+00 | 442 |
| 11.5 | 11.5 | 2413.613  | R | 0 | 2 | 1011.51 | 32622.320 | 3066.6952 | 5.055E-01 | 5.055E-01 | 3.167E-19 | 2.317E+04 | 0.31010E-01 | 443 |
| 7.5  | 7.5  | 1026.730  | R | 0 | 2 | 10.7.51 | 32623.600 | 3066.3741 | 1.005E+00 | 1.005E+00 | 6.000E-19 | 6.035E+04 | 1.09322E+00 | 444 |
| 12.5 | 11.5 | 2413.613  | R | 0 | 1 | 1011.51 | 32624.137 | 3066.2305 | 6.424E+00 | 6.424E+00 | 4.020E-10 | 2.610E+05 | 1.09040E+01 | 445 |
| 0.5  | 7.5  | 1026.730  | R | 0 | 1 | 10.7.51 | 32625.569 | 3066.1900 | 6.573E+00 | 6.573E+00 | 4.119E-10 | 2.604E+05 | 1.09040E+01 | 446 |
| 10.5 | 10.5 | 2015.036  | R | 0 | 2 | 1010.51 | 32626.901 | 3063.9710 | 6.209E-01 | 6.209E-01 | 3.092E-19 | 2.742E+04 | 0.91565E-01 | 447 |
| 0.5  | 0.5  | 1321.252  | R | 0 | 2 | 10.0.51 | 32627.304 | 3063.9256 | 9.099E-01 | 9.099E-01 | 3.953E-04 | 3.953E+04 | 1.01013E+00 | 448 |
| 9.5  | 9.5  | 1650.796  | R | 0 | 2 | 10.0.51 | 32628.072 | 3063.7059 | 7.552E-01 | 7.552E-01 | 4.733E-19 | 3.274E+04 | 0.51013E-01 | 449 |
| 11.5 | 10.5 | 2015.036  | P | R | 1 | 1010.51 | 32630.510 | 3063.7260 | 6.722E+00 | 6.722E+00 | 4.213E-10 | 2.722E+05 | 9.06003E+00 | 450 |
| 9.5  | 0.5  | 1321.252  | R | 0 | 1 | 10.0.51 | 32630.565 | 3063.7200 | 6.029E+00 | 6.029E+00 | 4.200E-10 | 2.671E+05 | 7.70050E+00 | 451 |
| 10.5 | 9.5  | 1650.796  | R | 0 | 1 | 10.0.51 | 32632.269 | 3063.5600 | 6.004E+00 | 6.004E+00 | 4.309E-10 | 2.707E+05 | 0.82700E+00 | 452 |
| 20.5 | 20.5 | 13005.249 | S | R | 2 | 1020.51 | 32633.357 | 3063.4500 | 1.337E-03 | 1.337E-03 | 0.307E-22 | 0.074E+02 | 1.79030E-01 | 453 |
| 2.5  | 1.5  | -056      | S | R | 2 | 10.1.51 | 32643.295 | 3062.5260 | 2.672E-01 | 2.672E-01 | 1.674E-19 | 2.305E+04 | 1.07007E-01 | 454 |
| 3.5  | 2.5  | 81.920    | S | R | 2 | 10.2.51 | 32696.505 | 3057.7249 | 4.135E-01 | 4.135E-01 | 2.592E-19 | 2.756E+04 | 2.90634E-01 | 455 |
| 20.5 | 27.5 | 17000.797 | S | 0 | 2 | 1027.51 | 32707.232 | 3056.5390 | 1.927E-03 | 1.927E-03 | 1.200E-21 | 1.000E+03 | 1.01036E-01 | 456 |
| 4.5  | 3.5  | 202.370   | S | R | 2 | 10.3.51 | 32744.561 | 3053.0564 | 4.629E-01 | 4.629E-01 | 2.901E-19 | 2.569E+04 | 3.40030E-01 | 457 |
| 27.5 | 26.5 | 12130.244 | S | 0 | 2 | 1026.51 | 32773.962 | 3050.3154 | 2.745E-03 | 2.745E-03 | 1.721E-21 | 1.140E+03 | 1.02567E-01 | 459 |
| 5.5  | 6.5  | 355.900   | S | R | 2 | 10.4.51 | 32792.722 | 3049.5704 | 4.564E-01 | 4.564E-01 | 2.063E-19 | 2.221E+04 | 3.63309E-01 | 459 |
| 26.5 | 25.5 | 11290.532 | S | R | 2 | 1025.51 | 32833.743 | 3044.7615 | 3.003E-03 | 3.003E-03 | 2.421E-21 | 1.204E+03 | 1.04451E-01 | 460 |
| 6.5  | 5.5  | 544.009   | S | 0 | 2 | 10.5.51 | 32830.395 | 3044.3301 | 4.219E-01 | 4.219E-01 | 2.644E-19 | 1.073E+04 | 3.59496E-01 | 461 |
| 25.5 | 24.5 | 10002.500 | S | R | 2 | 1024.51 | 32801.122 | 3040.3740 | 3.746E-01 | 3.746E-01 | 2.354E-19 | 1.569E+04 | 3.67219E-01 | 462 |
| 0.5  | 7.5  | 1029.092  | S | R | 2 | 10.7.51 | 32920.544 | 3039.0824 | 5.910E-03 | 5.910E-03 | 3.379E-21 | 1.440E+03 | 1.06713E-01 | 463 |
| 9.5  | 0.5  | 9491.321  | S | R | 2 | 1023.51 | 32933.211 | 3035.5650 | 7.625E-03 | 7.625E-03 | 4.654E-21 | 1.622E+03 | 1.09302E-01 | 465 |
| 9.5  | 0.5  | 1326.291  | S | R | 2 | 10.0.51 | 32956.371 | 3033.4317 | 2.793E-01 | 2.793E-01 | 1.751E-19 | 1.115E+04 | 3.15300E-01 | 466 |
| 23.5 | 22.5 | 0925.622  | S | 0 | 2 | 1022.51 | 32973.264 | 3031.0775 | 1.013E-03 | 1.013E-03 | 6.350E-21 | 1.019E+03 | 1.92591E-01 | 467 |
| 14.5 | 9.5  | 1654.577  | S | R | 2 | 10.9.51 | 32909.360 | 3030.4901 | 2.354E-01 | 2.354E-01 | 1.674E-19 | 9.494E+03 | 2.99633E-01 | 468 |
| 22.5 | 21.5 | 0806.350  | S | R | 2 | 1021.51 | 33007.099 | 3020.7695 | 1.370E-02 | 1.370E-02 | 0.500E-21 | 2.041E+03 | 1.95077E-01 | 469 |
| 11.5 | 10.5 | 2019.633  | S | R | 2 | 1010.51 | 33616.299 | 3327.9254 | 1.462E-01 | 1.462E-01 | 1.234E-19 | 0.143E+03 | 2.05026E-01 | 470 |
| 21.5 | 20.5 | 7474.376  | S | R | 2 | 1020.51 | 33034.000 | 3026.2215 | 1.031E-02 | 1.031E-02 | 1.140E-20 | 2.206E+03 | 2.00105E-01 | 471 |
| 12.5 | 11.5 | 2419.001  | S | R | 2 | 1011.51 | 33639.999 | 3025.7514 | 1.619E-01 | 1.619E-01 | 1.014E-19 | 7.035E+03 | 2.71673E-01 | 472 |
| 20.5 | 19.5 | 6790.692  | S | 0 | 2 | 1019.51 | 33056.060 | 3024.2155 | 2.626E-02 | 2.626E-02 | 1.520E-20 | 2.565E+03 | 2.04045E-01 | 473 |
| 13.5 | 12.5 | 2052.605  | S | R | 2 | 1012.51 | 33059.200 | 3023.9007 | 1.320E-01 | 1.320E-01 | 0.274E-20 | 6.111E+03 | 2.59626E-01 | 474 |
| 19.5 | 10.5 | 6135.500  | S | R | 2 | 1010.51 | 33073.060 | 3022.7341 | 3.101E-02 | 3.101E-02 | 1.994E-20 | 2.001E+03 | 2.10176E-01 | 475 |
| 16.5 | 13.5 | 3319.355  | S | 0 | 2 | 1013.51 | 33073.974 | 3022.6451 | 1.067E-01 | 1.067E-01 | 6.644E-20 | 5.330E+03 | 2.40029E-01 | 476 |
| 10.5 | 17.5 | 5510.159  | S | R | 2 | 1017.51 | 33003.652 | 3021.7604 | 4.132E-02 | 4.132E-02 | 2.590E-20 | 3.241E+03 | 2.14103E-01 | 477 |
| 15.5 | 14.5 | 3019.156  | S | 0 | 2 | 1014.51 | 33003.913 | 3021.7345 | 0.541E-02 | 0.541E-02 | 5.353E-20 | 4.607E+03 | 2.39107E-01 | 478 |
| 17.5 | 16.5 | 4915.197  | S | 0 | 2 | 1016.51 | 33040.916 | 3021.2001 | 5.316E-02 | 5.316E-02 | 3.332E-20 | 3.655E+03 | 2.22962E-01 | 479 |
| 16.5 | 15.5 | 4351.310  | S | 0 | 2 | 1015.51 | 33000.952 | 3021.2764 | 6.746E-02 | 6.746E-02 | 4.241E-20 | 4.129E+03 | 2.30590E-01 | 480 |

THE INTEGRATED INTENSITY FOR THE BAND IS 0.40629E+32 CM-2 ATM-1 AT T = 4600.0 K OR 5.46636E-16 CM/MOLECULE

ignored, our line strengths are identical to those calculated using Earls' formulas. Ignoring these effects does not significantly alter the line strengths for main branch transitions but does lead to large errors at high  $J$  for the weaker satellite branch line strengths. Earls' formulas (which ignore centrifugal and higher distortion and  $\Sigma$ - $\Pi$  interactions) predict consistently smaller line strengths than those calculated by us (which include centrifugal and higher distortion and  $\Sigma$ - $\Pi$  interactions). In the  $^2R_{12}$  branch, Earls' line strengths range from 93% of our line strength at  $J'' = 20.5$  to 69% of our line strength at  $J'' = 40.5$ ; in the  $^2R_{21}$  branch they range from 78% of our line strength at  $J'' = 20.5$  to 46% of our line strength at  $J'' = 39.5$ . Earls' formulas show intermediate error in this range for the other satellite branches.

Bennett's<sup>13</sup> line-strength formulas, which include  $P^4$  centrifugal distortion, may be expected to give much more accurate results. Based on our check of Earls' formulas, the line strengths for the  $^2R_{21}$  branch should have the largest deviation. Bennett's formula predicts line strengths for this branch which are 1% higher than ours at  $J = 1.5$  and decrease to 6% lower at  $J = 25.5$ ; they increase to 2% higher at  $J = 39.5$ . Examination of the eigenvectors shows that the  $P^4$  term and, to a lesser extent, the  $^2\Sigma$ - $^2\Pi$  mixing can contribute an effect of a few percent to the satellite bands line strengths. Thus, the dominant effect in the deviations from Earls' formulas is due to the centrifugal distortion, which is relatively large in a light molecule such as OH.

The conclusion to be drawn from these comparisons is that both the algebraic formulas or our method give accurate main branch line strengths at all experimentally observed  $J$  values. Earls' formulas lead to significant errors at high  $J$  in the satellite bands. Bennett's formulas give acceptable satellite branch line strengths for most work. However, when the highest accuracy is required, the line strengths from Table 9 should be used.

When our Einstein  $A$  coefficients are normalized to the same relative value as those of Chidsey and Crosley,<sup>1</sup> the two sets of values differ by at most  $\pm 2$  in the last decimal place. As with line strengths, these differences become important only at high  $J$  in the satellite branches where many of the relative Einstein  $A$  coefficients are quoted to only one significant digit by Chidsey and Crosley. An additional advantage of our Einstein  $A$  coefficients in Tables 8 and 9 for quantitative spectroscopy is that they are absolute rather than relative values.

Although we have chosen to present OH line parameters for temperatures of 240 and 4600°K, our computer program can generate  $A^2\Sigma$ - $X^2\Pi(0,0)$  band line parameters for any temperature. Table 10 may be used with Tables 8 or 9 and Eqs. (3) and (5) to convert line intensities from these temperatures to any temperature in the 200-6000°K range. Intensities so determined should have the same accuracy as those in Tables 8 and 9. Band intensities at temperatures other than 240 and 4600°K may be calculated by summing the individual line intensities at the desired temperature. Simpler approximate procedures which directly convert from a band intensity at one temperature to a band intensity at another temperature such as Eq. (7-126) in Penner,<sup>6</sup> give errors of approx. 15% when band intensities at 240 and 4600°K are compared.

Table 10. Rotational partition function  $Q_R$  vs temperature  $T$ .

| $T$ (K) | $Q_R$  | $T$ (K) | $Q_R$  |
|---------|--------|---------|--------|
| 200     | 26.71  | 2000    | 298.23 |
| 240     | 32.24  | 2500    | 373.27 |
| 296     | 40.17  | 3000    | 454.19 |
| 300     | 40.75  | 3500    | 533.18 |
| 500     | 70.00  | 4000    | 612.85 |
| 750     | 107.35 | 4500    | 693.14 |
| 1000    | 145.09 | 4600    | 709.26 |
| 1250    | 183.08 | 5000    | 773.98 |
| 1500    | 221.28 | 5500    | 855.28 |
| 1750    | 259.67 | 6000    | 936.88 |

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## ERRATUM

The following corrections should be made to Goldman and Gillis<sup>1</sup>.  
In Eq. (3) and (7) the expression  $(2J'+1)$  should be  $4(2J'+1)$ .  
Consequently, all intensities in  $\text{cm}^{-1}/\text{atm-cm}$  and  $\text{cm}/\text{molecule}$  in Ref. 1  
should be multiplied by 4. All other line parameters remain unchanged.

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