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AIR FORCE CAMBRIDGE RESEARCH LABORATORIES
L. G. HANSCOM FIELD, BEDFORD, MASSACHUSETTS

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AIR FORCE SYSTEMS COMMAND
United States Air Force

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R.A. McCLATCHEY
W.S. BENEDICT [*]
S.A. CLOUGH
D.E. BURCH [†]
R.F. CALFEE
K. FOX [‡]
L.S. ROTHMAN
J.S. GARING

[*] University of Maryland
[†] Philco Ford Corporation
[‡] University of Tennessee

AIR FORCE SYSTEMS COMMAND
United States Air Force

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R.A. McClatchey	D.E. Burch	L.S. Rothman
W.S. Benedict	R.F. Calfee	J.S. Garing
S.A. Clough	K. Fox	

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13. ABSTRACT

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A discussion is provided separately for each molecular species, indicating the sources and accuracy of the data and a general discussion of how the data were obtained.

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Abstract

The report describes a compilation of the molecular spectroscopic parameters for a number of infrared-active molecules occurring naturally in the terrestrial atmosphere. The following molecules are included in this compilation: water vapor; carbon dioxide; ozone; nitrous oxide; carbon monoxide; methane; and oxygen. The spectral region covered extends from less than 1 μm to the far infrared, and data are presented on more than 100,000 spectral lines. The parameters included in the compilation for each line are: frequency, intensity, half-width, energy of the lower state of the transition, vibrational and rotational identifications of the upper and lower energy states, an isotopic identification, and a molecular identification.

A discussion is provided separately for each molecular species, indicating the sources and accuracy of the data and a general discussion of how the data were obtained.

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AFCRL Atmospheric Absorption Line Parameters Compilation

1. INTRODUCTION

About 10 years ago a program was initiated to compile spectroscopic data on individual vibration-rotation lines of water vapor in the 2.7 μm region (Gates, et al, 1964).

This work continued resulting in a publication on the 2.05 and 2.7 μm bands of carbon dioxide (Calfee and Benedict, 1966) and a third publication on the 1.9 and 6.3 μm bands of water vapor (Benedict and Calfee, 1967). Other workers have published similar results on the 15 μm bands of CO_2 (Drayson and Young, 1967), the 9.6 μm bands of O_3 (Clough and Kneizys, 1965), the CO bands whose fundamental is near 5 μm (Kunde, 1967), the CH_4 bands near 3 and 7.5 μm (Kyle, 1968) and the unpublished rotational water data calculated by Benedict and Kaplan in 1959 (see Goody, 1964, p. 184).

About 5 years ago an effort was initiated at AFCRL to continue this work with the aim of providing a complete set of data for all vibration-rotation lines of all naturally occurring molecules of significance in the terrestrial atmospheres. With such data at hand, it would be possible to compute the transmittance appropriate for atmospheric paths by first computing the monochromatic transmittance many times in a finely spaced frequency grid and then degrading the results to any appropriate spectral resolution. Up to now the following molecules have been included in this compilation: (1) water vapor; (2) carbon dioxide; (3) ozone; (4) nitrous oxide; (5) carbon monoxide; (6) methane; and (7) oxygen.

(Received for publication 26 January 1973)

All of these molecules except oxygen are minor constituents of the atmosphere, but nonetheless represent most of the absorption lines in the visible and infrared. Although there is some evidence for decreasing concentration with height of N_2O, CO, and CH_4, it is probably reasonable for most purposes to assume that all of these gases except H_2O, and O_3 are uniformly mixed by volume in the atmosphere unless other specific information is available. Table 1 provides concentrations and references for these "uniformly mixed gases". Water vapor and ozone are, of course, not uniformly mixed and an appropriate set of models useful in considering the radiation effects of these gases is provided by McClatchey, et al, 1972.

Table 1. Concentrations of Uniformly Mixed Gases in Dry Air

Constituent	ppm by volume	Reference
CO_2	330	Fink et al, 1964
N_2O	0.28	Birkland and Shaw, 1959
CO	0.075	Shaw, 1968
CH_4	1.6	Goody, 1964
O_2	2.10×10^5	Valley, 1965

2. DESCRIPTION OF COMPILATION

In order to compute the transmittance due to a given spectral line in the atmosphere it is necessary to describe the absorption coefficient as a function of frequency for each line. The four essential line parameters for each line are the resonant frequency, ν_o(cm^{-1}), the intensity per absorbing molecule, S(cm^{-1}/molecule cm^{-2}) the Lorentz line width parameter, α_o(cm^{-1}/atm), and the energy of the lower state, E″(cm^{-1}). The frequency, ν_o, is independent of both temperature and pressure (except for possibly very small pressure effects of less than 0.01 cm^{-1}/atm, which have been ignored here). The intensity, S, is pressure-independent, and, as discussed below, its temperature dependence can be calculated from E″ and ν

The line half-width at half maximum, α, is by definition proportional to the pressure, p, and its temperature dependence can be estimated as discussed below.

The precise line shape is a matter of some uncertainty, but in the derivation of line parameters from laboratory measurements, it is customary to start from the Lorentz shape (see Goody, 1964) given in Eq. (1).

$$k(\nu) = \frac{S\alpha}{\pi(\nu - \nu_o)^2 + \alpha^2} \tag{1}$$

$$S = \int k(\nu)\, d\nu$$

The validity of Eq. (1) to describe the true line shape is subject to two limitations. The first, which can be precisely estimated and corrected for by the use of the Voigt shape, occurs when $\alpha_o P/\alpha_D < 1.0$ where α_D is the doppler line width which varies with frequency, temperature and molecular mass as given in Eq. (2).

$$\alpha_D = \frac{\nu}{c}\left(\frac{2kT \, \ln 2}{m}\right)^{1/2} = 4.298 \times 10^{-7} \nu (T/M)^{1/2} \qquad (2)$$

where M = molecular weight and here k = Boltzmann's constant and m = mass of a molecule.

For atmospheric molecules and infrared frequencies, modifications of the Lorentz shape begin to be required at pressures below 10 to 100 mb.

The second limitation concerns possible inadequacies of the Lorentz shape, especially in the distant wings of a line ($|\nu - \nu_o| >> \alpha$) (see Winters et al, 1964, and Burch et al, 1969) or when the long-range intermolecular forces responsible for collision broadening are dipole-quadrupole, leading to an exponent 1.75 rather than 2.0 for ($\nu - \nu_o$), (Varanasi, 1972). Throughout this compilation we assume the validity of the Lorentz exponent.

The line intensity is temperature dependent through the Boltzmann factor and the partition function as indicated in Eq. (3) (the induced emission term has intentionally been omitted here),

$$S(T) = \frac{S(T_s)\; Q_v(T_s)\; Q_r(T_s)}{Q_v(T)\; Q_r(T)} \; \exp + \left[\frac{1.439E'' \; (T-T_s)}{T\,T_s}\right] \qquad (3)$$

where E'' (in cm^{-1}) is the energy of the lower state of the transition and where Q_v and Q_r are the vibrational and rotational partition functions. The vibrational partition functions for the most abundant isotopes are given in Table 2. Partition functions for the other isotopes are similar. The temperature dependence of the rotational partition function is given by $(T/T_s)^j$ where j is also provided in Table 2 (T_s is taken to be 296°K).

It is also necessary to know the temperature variation of α. In the absence of specific indications discussed under each molecule, the equation $\alpha(T)/\alpha(T_s) = (T/T_s)^{-n}$, with n = 1/2, corresponding to the assumption of temperature-independent collision diameters, may be made. The validity of the assumption is more uncertain, the larger the dependence of the diameter on the particular rotation-vibration transition, (that is, it is most unrealistic for H_2O and the low-J transitions of the other molecules). The theory of Tsao and Curnutte (1954) when applied to the determination of line width for H_2O lines gives a wide variation of n about the mean value of 0.62 (Benedict and Kaplan, 1959). Measurements made with a CO_2 laser (Ely and McCubbin, 1970) indicate a value of n = 1.0 for the P20 line of the 10.4 μm CO_2 band.

Table 2. Vibrational Partition Functions

Molecule	j	Temperature	175	200	225	250	275	296	325
H_2O	1.5		1.000	1.000	1.000	1.000	1.000	1.000	1.001
CO_2	1.0		1.0095	1.0192	1.0327	1.0502	1.0719	1.0931	1.1269
O_3	1.5		1.004	1.007	1.013	1.022	1.033	1.046	1.066
N_2O	1.0		1.017	1.030	1.048	1.072	1.100	1.127	1.170
CO	1.0		1.000	1.000	1.000	1.000	1.000	1.000	1.000
CH_4	1.5		1.000	1.000	1.001	1.002	1.004	1.007	1.011
O_2	1.0		1.000	1.000	1.000	1.000	1.000	1.000	1.001

An examination of Eqs. (1) and (3) indicates that it is necessary to know the ν_o, $S(T_s)$, $\alpha(P_o, T_s)$ and E'' value for each line in order to compute a spectrum. The data compilation described here contains these four quantities for each of the more than 100,000 lines between 1 μm and the far infrared belonging to the seven molecular species listed in Table 3. Additional identifying information is also supplied for each line as indicated below.

Table 3. Intensity Criteria for Lines Included in Compilation

Molecule	Identification No.	Criterion Intensity* Minimum at T=296K	Existing Intensity Minimum at T=296K
H_2O	1	3×10^{-27}	3×10^{-27}
CO_2	2	2.2×10^{-26}	3.7×10^{-27}
O_3	3	3.5×10^{-24}	3.5×10^{-24}
N_2O	4	3.0×10^{-23}	4.0×10^{-23}
CO	5	8.3×10^{-23}	1.9×10^{-23}
CH_4	6	3.3×10^{-24}	3.3×10^{-24}
O_2	7	3.7×10^{-30}	3.7×10^{-30}

*Units are $cm^{-1}/(molecule\text{-}cm^{-2})$

In order to establish the "Criterion Intensity Minimum" values given in Table 3, an extreme atmospheric path was considered, assuming the gas concentrations specified in Table 1 and maximum concentrations over the path of 3×10^{24} molecules/cm^2 for water vapor and 1×10^{20} molecules/cm^2 for ozone. This extreme radiation path was the atmospheric path tangent to the earth's surface, and extending from space to space. Using this criterion, lines yielding less than 10 percent absorption at the line center would normally be omitted.

Although this absolute line intensity cutoff was established, it has not always been possible to achieve. In some cases it would have been unrealistic to push calculations to this limit when experimental confirmation fell far short. There are two specific areas in which this absolute cutoff has been violated: (1) In regions of very strong absorption, very weak lines above this absolute limit have been neglected; (2) Q-branch lines below this limit have occasionally been included where it is felt that the accumulation of many weak, closely spaced lines would still produce an appreciable absorption under some atmospheric circumstances. In some cases, (for example, CO_2), sufficient laboratory measurements and theoretical work were available so that this limit was exceeded throughout the infrared.

In the past, line intensities have been defined in various units, different for each molecular species. It was common to define water vapor concentration in precipitable cm, or g/cm^2, in the path in question. On the other hand, the amount of CO_2 and the other uniformly mixed gases in a path were often given in cm-atm of gas at STP. In order to unify the units and ultimately to lead to less confusion, we decided to use the more fundamental quantity, molecules/cm^2 as a measure of absorbing gas abundance along the path. The appropriate conversion factors are:

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

$$1\ \text{g/cm}^2 \text{ of } H_2O = 3.34 \times 10^{22}\ \text{molecules/cm}^2 .$$

It was also decided, as indicated in Table 3, to define line (and band) intensities at $296^{\circ}K$, the normal room temperature at which most measurements are made. Intensities of all bands are based on the total number of molecules of a given species of all isotopes in their normal abundance, not on the number of the particular isotope responsible for a given band. Isotopic abundance values for all molecules for which data are provided in the compilation are given in Table 4.

Half-widths of lines have been added where available. Details are discussed in the separate sections on individual molecules. In some cases, it is felt that insufficient data exist to warrant the inclusion of a variable half-width. In these cases, a mean, constant value has been inserted for each molecular species and values are given in Table 5.

A shorthand notation was adopted to identify the various isotopic species. It is easy to understand by considering the following examples for CO_2: ${}^{16}O^{12}C^{16}O \equiv 626$, ${}^{16}O^{13}C^{16}O \equiv 636$, and for N_2O, ${}^{14}N^{15}N^{16}O \equiv 456$, etc. This same type of code is used for the other five molecules.

Table 4. Isotopic Abundances

H_2O	161	0.99729	CH_4	211	0.98815
	162	0.000300		311	0.01110
	181	0.00204	CH_3D	212	0.00060
	171	0.000370			
CO_2	626	0.98414	O_2	66	0.99519
	636	0.01105		68	0.00407
	628	0.00402		67	0.00074
	627	0.000730			
	638	0.0000452			
	637	0.00000820			
	828	0.00000412			
O_3	666	0.99279			
	668	0.00406			
	686	0.00203			
N_2O	446	0.99022			
	456	0.00368			
	546	0.00368			
	448	0.00202			
	447	0.00037			
CO	26	0.98652			
	36	0.01107			
	28	0.00202			
	27	0.000369			

Table 5. Mean Half-width Values

Molecule	Half-width (cm^{-1}/atm)	References
CO_2	0.07	Yamamoto et al (1969)
$O3$	0.11	Lichtenstein et al (1971)
N_2O	0.08	Toth (1971)
CO	0.06	Bouanich and Haeusler (1972)
CH_4	0.055	Varanasi (1971) (see Section 6.3)
O_2	0.060	Burch and Gryvnak (1969)

A standard computer format was adopted for card or card-image input and is outlined below, the numbers between vertical lines representing the columns on an IBM card, and the letter-number combinations representing the computer format.* The first four quantities are: ν = frequency in

ν	S	α	E''	Rotation and Vibration ID	Date	Isotope	Molecule
1-10	11-20	21-25	26-35	36-70	71-73	74-77	78-80
F10.3	E10.3	F5.3	F10.3	5A6, A5	I3	I4	I3

---

*In the far infrared ($\nu < 100$ cm^{-1}) a different format (F10.6) was occasionally chosen for the frequencies where high accuracy microwave measurements are available.

wavenumbers, S = line intensity in $cm^{-1}/molecule\text{-}cm^{-2}$ at 296°K, α = half-width in cm^{-1} atm at 296°K, E'' = energy of the lower state expressed in wavenumbers. The rotation and vibration identification are the most difficult to unify due to the differences in the quantum numbers required to define the upper and lower states for different kinds of molecules. The columns 36 through 70 are indicated below for water and ozone, both triatomic asymmetric molecules, where (') indicates upper state and ('') indicates the lower state.

J', K_a', K_c'		J'', K_a'', K_c''		$v'_1v'_2v'_3$		$v_1''v_2''v_3''$	
3I3	1X	3I3	2X	3I2	1X	3I2	1X

On the other hand, the quantum numbers specified for CO_2 and N_2O between columns 36 and 70 are given below, where again (') indicates upper state and ('') indicates lower state, and where r refers to Fermi resonance (see section on CO_2 for more details). The identification system for methane differs from those described here and is described in the section on methane.

	$v'_1v'_2\ell'v'_3r'$		$v''_1v''_2\ell''v''_3r''$	P(J'' + 1)
2x		5x	5I2	A8

The remaining fields specified above include the entry date of the datum (important primarily for our purposes), the isotopic code as described above, and the molecular identification as given in Table 3.

This work has now proceeded to the point where most of the data consistent with the above-mentioned line intensity limitation are fairly complete in the 1 μm to 100 μm region. The nature of the remaining uncertainties and omissions is discussed in the sections to follow. The data are frequency ordered on magnetic tape and are contained in records of 321 ten-character words per record. An initial control word indicates the number of words to follow (320 for a full record). Each such record contains 40 card images in the format described above. Thus, it is necessary after reading a record from the tape to decode it according to the format I10, 40 (F10.3, E10.3, F5.3, F10.3, 5A6, A5, I3, I4, I3). In order to aid those using other than Control Data Corporation equipment, Table 6 is provided. The column headed "External BCD Code" indicates the character representation actually used on the tape. If a computer having a different character code is being used, a simple cross-referencing program must be constructed. End of file markers are placed on the tape at the following frequency points: 500, 1000, 2500, 5000, 10,000 cm^{-1} with a double end of file appearing at the end of the tape.

In Appendix A we have included a listing of a computer program for directly reading the tape on a CDC 6600 computer. (No card decks are available.) For other computer systems the used is left to his own devices. Appendix B provides a computer program and output for generating a synthetic spectrum for a constant pressure path.

Table 6. CDC 6000 Series Fortran Character Codes*

Source Language Character	Console Display Code	External BCD Code	Punch Position in a Hollerith Card Column
A	01	61	12-1
B	02	62	12-2
C	03	63	12-3
D	04	64	12-4
E	05	65	12-5
F	06	66	12-6
G	07	67	12-7
H	10	70	12-8
I	11	71	12-9
J	12	41	11-1
K	13	42	11-2
L	14	43	11-3
M	15	44	11-4
N	16	45	11-5
O	17	46	11-6
P	20	47	11-7
Q	21	50	11-8
R	22	51	11-9
S	23	22	0-2
T	24	23	0-3
U	25	24	0-4
V	26	25	0-5
W	27	26	0-6
X	30	27	0-7
Y	31	30	0-8
Z	32	31	0-9
0	33	12	0
1	34	01	1
2	35	02	2
3	36	03	3
4	37	04	4
5	40	05	5
6	41	06	6
7	42	07	7
8	43	10	8
9	44	11	9
+	45	60	12
-	46	40	11
*	47	54	11-8-4
/	50	21	0-1
(	51	34	0-8-4
)	52	74	12-8-4
$	53	53	11-8-3
=	54	13	8-3
blank(space)	55	20	space
,	56	33	0-8-3
.	57	73	12-8-3

*Taken from Control Data 6400/6500/6600 Fortran Reference Manual, Publication No. 60174900 Rev. C (1968) Control Data Corporation

Interested parties can obtain a copy of the data tape described here by mailing a new, 7-track, 800 BPI certified, 2400 ft long by 1/2 in. wide, magnetic tape to R. A. McClatchey, AFCRL (OPI), L. G. Hanscom Field, Bedford, Ma. 01730.

Due to the large amount of material included on this tape and the likelihood of errors, it is clear that the ultimate test of the accuracy and completeness of the data will be its use by many people in the scientific community. Therefore, we ask the cooperation of all who use these data to keep us informed of any apparent errors or omissions. We would appreciate the receipt of new laboratory data or theoretical work related to improving the data. We will then update this tape as sufficient new or revised data become available.

3. GENERAL REMARKS ON THE DERIVATION OF PARAMETERS

The four tabulated parameters, ν_o, E'', S, and α must of course be derived from experimental observations, subjected to data reduction in the framework of the general theories of molecular spectroscopy. For the basic theory we refer the reader to such textbooks as Herzberg (1950) and Goody (1964). The complexity needed to approach the problem depends both on the type of molecule and the accuracy of the observational data. We here outline the equations and methods used for the general types of molecules, linear triatomic (and diatomic) CO_2, N_2O and (CO); nonlinear triatomic, H_2O and O_3. Methane, CH_4, a spherical top, is a special case, as is the diatomic O_2, where unpaired electrons complicate the rotational structure of the ground and excited electronic states.

The energy states and the transition probabilities between energy states of the molecules are defined primarily by their numerical values as established by experiments and by the indices (quantum numbers) which identify them. In nearly all the cases of interest, mathematical relations of greater or lesser complexity relate the numerical properties to the quantum numbers. We here present the general relations used to generate the tabulated data. The specific data and exceptional cases are discussed later for each molecule.

3.1 Energy Levels and Line Positions

3.1.1 LINEAR MOLECULES

For the triatomic linear molecules CO_2 and N_2O, the vibrational states are characterized by three quantum numbers, which are zero or positive integers, of pure vibration, v_1, v_2, and v_3 and a fourth number $\ell_2 = v_2, v_2 - 2 \ldots$ which represents the contribution of the bending mode to the angular rotation. In order to calculate the purely vibrational part of the energy ("the band origins"), it is necessary first to compute an unperturbed energy,

$G_v{}^{unp}$, by: $$G_v{}^{unp} = \sum_i \omega_i{}^{vi} + \sum_{ij} X_{ij} v_i v_j + g_{22} \ell^2 + \sum_{ijk} v_i v_j v_k + \sum_{ijk} v_i \ell^2 + \ldots \qquad (4)$$

and then to incorporate the effects of resonance perturbation by combining all close-lying levels with common ℓ and common symmetry in matrices whose diagonal elements are $G_v{}^{unp}$, whose off-diagonal elements are functions of additional molecular constants and the four quantum numbers, and whose eigenvalues are the vibrational energy G_v. For an excellent discussion and example, the reader is referred to the work on N_2O by Pliva (1968).

This perturbation calculation results in the "mixing" of states whose $G_v{}^{unp}$ are particularly close, so that the final description of the level by the original four quantum numbers is a poor one. Accordingly, it is useful to add a fifth index, the rank symbol r to label in order of decreasing energy all such mixed states. We have adopted this procedure for CO_2, where the mixed states are $(v_1\ v_2\ \ell_2\ v_3)$, $(v_1 + 1, v_2 - 2, \ell_2, v_3)$, . . . etc. The highest value of v_1 and the lowest value of v_2 in each set are retained in the vibrational indentification for all levels of the set.

In the present compilation, the above method was used to generate those energy levels which have not been observed; for all observed states the experimental value (averaged from various sources) was used.

The rotational energy of each vibrational state is given by:

$$E_{v,j} = G_v + B_v \left[J(J+1) - \ell^2\right] - D_v \left[J(J+1) - \ell^2\right]^2 + H_v \left[J(J+1) - \ell^2\right]^3 + \ldots, \qquad (5)$$

where the constants B_v, D_v, H_v for each vibrational state are either determined by observation or calculated from a smaller number of rotational molecular constants. Whenever accurate constants have been observed, these are used; calculated values are reserved for the less important states. The equations for calculations of B_v and D_v are similar to those for G_v, and likewise require modification through the resonance perturbation. Evaluation from data of the small H_v constants requires highly accurate measurements extending to high J, so that in most cases these are fixed at zero; the non-zero values arise from resonances.

It will be noted in Eq. (4) that the vibrational energy depends on ℓ^2. When $\ell \neq 0$ there are two levels for each $J \geq \ell$, and this degeneracy is removed by rotation. The splitting ("ℓ-type doubling") results in two sets of levels, designated c and d, with different effective rotational constants. When $\ell = 1$ the splitting is most important, and $B_c \neq B_d$, $D_c \neq D_d$, etc.; when $\ell = 2$, $B_c = B_d$ but $D_c \neq D_d$, etc.; when $\ell = 3$, the constants other than H are the same. Resonances occasionally cause larger deviations.

When the linear molecule has a center of symmetry, as in CO_2 with ^{16}O at both ends (but not when one oxygen is isotopically different), the paired atoms with zero nuclear spin cause zero statistical weight for rotational levels of a given parity. Thus, only even-J levels exist for the ground vibrational level and for all other levels with $\ell = 0$ and v_3 even ("Σ_g^+ symmetry"); for levels with $\ell = 0$ and v_3 odd (Σ_u^-), only J odd exists; when $\ell > 0$, the c- and d- sublevels have different symmetry, so that for $\ell = 1(\pi_g)$ the J = odd levels are c and the J = even levels are d, etc. In the compilation symbols c or d are appended to the rotational quantum number of the lower state only when required, that is for $\ell \geq 1$ in the molecules without the center of symmetry. For example, R27C means 28c ← 27c; Q27C means 27d ← 27c.

The line frequencies are determined from the energy states by taking the differences corresponding to all allowed transitions. These depend on the familiar selection rules for the linear molecule:

When $\Delta \ell = 0, \Delta J = \pm 1$, c ↔ c, d ↔ d.
When $\Delta \ell = 1, \Delta J = \pm 1$, c ↔ c, d ↔ d,
and $\Delta J = 0$ c ↔ d.

The line positions may thus be conveniently represented for computational purposes as given series in <u>m</u>, where $m = J'' + 1$ for the R-branch ($J'' \rightarrow J''+1$), $m = -J''$ for the P-branch ($J'' \rightarrow J''-1$), and $m = J''$ for the Q-branch ($J'' \rightarrow J''$). A different equation is needed for Q-branch of a given transition than for the P and R branches, because of the differences in the <u>c</u> and <u>d</u> constants. The general equation is

$$\nu(m) = G_v + am + bm^2 + cm^3 + dm^4 + em^5 + fm^6, \text{ with } a = (B'_v + B''_v);$$

$$b = (B'_v - B''_v - D' + D''); \; c = -2(D'_v + D''_v); \; d = -(D'_v - D''_v);$$

$$e = 3(H'_v + H''_v); \; f = (H'_v - H''_v). \tag{6}$$

3.1.2 NONLINEAR MOLECULES

The nonlinear triatomic molecules H_2O and O_3 have similar basic structures. The formula for the vibrational energy is identical with Eq. (4), except that the quantum number ℓ and its associated constants do not exist. Vibrational resonances exist; in both H_2O and O_3, $\omega_1 \sim \omega_3$, but these are of different symmetry, so that interaction between the band origins and identical rotational states occurs only in (200,002), etc. In addition for H_2O, and much more closely for the 162 isotope, $2\omega_2 \approx \omega_1$, so that the properties of the higher vibrational levels must be computed by taking their resonances into account.

The rotational levels of these three-dimensional rotators, with three different reciprocal moments of inertia $A_v > B_v > C_v$ are labelled by three quantum numbers, J, K_a, K_c, with K_a and K_c assuming all values 0, 1, . . . J, subject to $K_a + K_c = J$ or $J + 1$. There are thus $2J + 1$ levels of a given J (each again with a rotational statistical weight of $2J + 1$); in addition there is a nuclear-spin statistical weight which gives alternate levels, depending on the odd or even parity of $J+K_a+K_c+v_3$, weights of 3 or 1 for H_2O, 0 or 1 for isotopically symmetrical O_3. The normal progressions of energy within each J is increasing with increasing K_a-K_c; occasionally inversions of a few paired levels may occur in excited vibrational states as a result of rotation-vibration interactions between close-lying states of like over-all symmetry in different vibrational levels. As J increases, there is a tendency for the odd and even levels with K_a or K_c close in value to J to approach very closely in energy, so that many apparently single lines are in reality degenerate pairs with unresolvable spacings. The range of K_a, K_c in which these pairings occur, and the general spacing of the rotational levels is governed by the asymmetry parameter, $\kappa = (2B-A-C)/(A-C)$, which for the ground vibrational states of H_2O, HDO, O_3 is respectively -0.437, -0.689, and -0.984. As the parameter approaches -1, the energy level formula approaches that of the symmetric top with $A > B = C$ namely,

$$E_r = \frac{B+C}{2} J(J+1) + \left(A - \frac{B+C}{2}\right) K_a^2 - D_J J^2 (J+1)^2 - D_{JK} J (J+1) K^2 - D_K K^4 \tag{7}$$

where the D's are centrifugal stretching constants, and where additional terms of powers higher in J^2, K^2 are often required. For the asymmetric top molecules with $K \neq -1$, the rotational energy cannot be given by a closed formula, but requires the construction and diagonalization of matrices whose diagonal elements are given by Eq. (7) whose off-diagonal elements involve B-C and two additional centrifugal stretching constants of power 4, etc., and whose eigenvalues are the rotational energy. From the eigenvectors of the diagonalization, one obtains effective angular moments about each axis, $\langle P_a^2 \rangle$, $\langle P_b^2 \rangle$, $\langle P_c^2 \rangle$, whose sum, $P^2 = J(J+1)$ and one also obtains other coefficients necessary for the calculation of transition probabilities and other properties of each eigenstate.

The excited vibrational levels of water vapor may differ considerably from the ground state in their values of A, B, and C, and with a relatively high ratio of A/ω_2 ($\simeq 0.018$, as contrasted to 0.00059 for B/ω_2 in CO_2), extensive overlapping occurs between rotational levels in nearby vibrational states, making the computation of the higher levels highly uncertain much beyond the limits of observation. Accordingly, for all except the lowest energy levels of the ground state it is preferable to use experimental rather than calculated values when available.

3.2 Line Intensities

The intensity of any line at frequency ν may be expressed in a purely formal way as:

$$S_m = \frac{\nu}{\nu_o} \cdot S^o_v \cdot S_{Rot} \cdot F \tag{8}$$

where S^o_v is the vibrational intensity of a nonrotating molecule at the vibrational origin, ν_o ; S_{Rot} is the rotational intensity for a rigid nonvibrating molecule and F is a factor that takes into account the fact that both forms of motion are occurring simultaneously. In the rigid case, F = 1, and if S_{Rot} is normalized so that $\Sigma_{Rot} S_{Rot} = 1$ and if the band extends over a limited frequency range so that $\nu/\nu_o \sim 1$, then S^o_v as defined by Eq. (8) is identical with the quantity usually denoted by S_v, the total band intensity, $\Sigma_m S_m$.

S_{Rot} consists of a temperature-independent factor, the rotational line strength, L_R, common to all linear molecules, and a temperature-dependent Boltzmann factor [Eq. (13)]. If the sum of all transitions from J" is normalized to the statistical weight g = 2J"+1, and if one recalls the definition of the rotational partition function $Q_r(T) = \Sigma g \exp(-1.439 E_R/T)$ (the summation is over all rotational levels of a given v), the normalization condition for all transitions $(\Sigma S_{Rot} = 1)$ is fulfilled.

The equations for L_R are as follows:

$\Delta \ell$	ΔJ	L_R	
0	0	$\ell^2(2m+1)/m(m+1)$	(9)
0	± 1	$(\lvert m\rvert - \ell^2)/\lvert m\rvert$	(10)
± 1	0	$(\lvert m\rvert + 1 \pm \ell)(m \mp \ell)(2m+1)/m(m+1)$	(11)
± 1	± 1	$(\lvert m\rvert \pm 1 \pm \ell)(\lvert m\rvert \pm \ell)/\lvert m\rvert$	(12)

Equation (8) is exact with F = 1 only for a rigid molecule. In the actual molecule, a number of factors may cause deviations, which however will vary regularly along the band. (A very few exceptional situations, "crossing perturbations", may also be recognized.) Depending on the precision of the measurements, the non-rigidity corrections ("F-factors") for the linear molecule, may be expressed as regular functions of the running index, m, as indicated in Eq. (13).

$$F = S_{nonrigid}/S_{rigid} = (1 + am + bm^2 \ldots) . \tag{13}$$

The first order theoretical correction is $F = (1 + \zeta m)^2$ or $a = 2\zeta$, $b = \zeta$. For nearly all the intensities in the present compilation, a single ζ was used for each vibrational band; this is included in the tabulations of band parameters. More refined measurements and theoretical calculations should, in future revisions of this compilation, permit the use of additional terms in Eq. (13).

For asymmetric top molecules, many more transitions are possible from each rotational level $J\ K_a K_c$, but the same general definitions hold. The values of L_{Rot} depend on the degree of asymmetry. Tabulations exist (Wacker, 1964) which are useful for orientation purposes. In the present work we either derive L_R from the rotational constants, for pure-rotation bands and some fundamental bands, or make use of the tables.

The F-factor corrections to the intensities become of considerable significance for most of the vibration-rotation transitions in H_2O. Various methods are used, based in part on theoretical considerations described later on, and in part on an arbitrary empirical adjustment of calculated values to the best observations.

A few general remarks should be made regarding the temperature dependence of $S_v{}^o$. $S_v{}^o$ is proportional to the product of the relative population of the lower state, given by the vibrational Boltzmann terms $\exp(-1.439\ G_v)/Q_v$, (with $Q_v \equiv \sum_v g_v \exp(-1.439 G_v)$ where g_v is the degeneracy of the level, 1 when $\ell = 0$, 2 otherwise), and a temperature independent transition probability, $u_{vv'} = |\int \widetilde{\Psi}_v u \psi_{v'}\, d\tau|^2$, ψ being the dipole moment function, usually expressed as a Taylor's series expansion in the dimensionless normal coordinates. We rely on measurement to give the total absorption strength in a given spectral region. When the spectral resolution is sufficiently high to distinguish lines of the strongest band in the region, usually the one with the lower level $v = 0$, from lines of all of the weaker "hot" or isotopic bands which accompany it, no problems arise: The S_v^o of each band, and accordingly the relative $\mu_{vv'}$ is empirically established (along with favorable cases a determination of coefficients of the F-factor, leading to ΣS_v for the region). However, most of the studies of quantitative band intensities have been made under conditions where only the total intensity is observed and the strengths of the weaker lines, which contribute only a few percent of the total, estimated from theoretical relations.

When all the transitions in the region are of the same type (that is, have identical Δv_1, Δv_2, Δv_3, $\Delta \ell$), a good approximation to the relative transition probability is to use harmonic oscillator wave functions and to assume that the leading term in the expansion of μ is formed by the Δv's: for example if $\Delta v_1 = 2$, $\Delta v_3 = 1$, we require that this term be $\mu_{113}\, q^2{}_1\, q_3$ with $\mu_{113} = \partial^3 \mu / \partial q_1{}^2 \partial q_3$. Evaluation of the integral for arbitrary values of $v_1, v_2, v_3 \rightarrow v_1 + 2, v_2, v_3 + 1$ then gives the ratio $\mu^2_{vv'}/\mu^2_{o\ 201} = (v_1 + 2)!\,(v_3 + 1)!/v_1!\,v_3!$. The general formula (for $\Delta \ell = 0$) is $(v_1 + \Delta v)!\,(v_2 + \Delta v)!\,(v_3 + \Delta v)!/v_1!\,v_2!\,v_3!$. When $\Delta \ell = \pm 1$ similar relations involving integers hold. Use of more realistic wave functions corrected for an harmonicity with lower terms in the dipole expansion lead to very nearly the same ratios. Accordingly, for many transition regions this type of calculation is simple and acceptable.

When, however, as in the case of both CO_2 and N_2O, the resonance perturbations mix the vibrational wavefunctions, a region includes several bands with different basic transitions. For example, the 1.6μ region of CO_2 contains four strong $\Delta \ell = 0$ bands, composing the resonance quartet 3001r-0, with r=1, 2, 3, 4. If we assume that only the $\Delta v_1 = 3$, $\Delta v_3 = 1$ transition is involved, the relative transition probability of the four transitions should be given by the squared eigenvectors of the $\{301, 221, 141, 061\}$ matrix, and the relative transition probability of the four hot transitions from 010 would be the same value (since $\Delta v_2 = 0$) multiplied by the squared eigenvectors of the $\{311, 231, 151, 071\}$ matrix. These are not identical with the other eigenvectors, and all four hot bands have different transition probabilities. Moreover, the observed ground-state intensities are not proportional to the first set of eigenvectors. Inclusion of a second basic transition integral for $\Delta v_1 = 2$, $\Delta v_2 = 2$, $\Delta v_3 = 1$, together with the appropriate eigenvectors can, however, bring the observations in accord with calculation, if the ratio μ_{221}/μ_{301} is of the order of 0.1. The ratio 231-0/221-010 is 3, and accordingly its inclusion increases the over-all -010/0 strength ratio and further shifts the relative probabilities. As one extends the calculations to lower states involving resonating groups with $v_2 = 2$, 3, and higher, required in the stronger bands of CO_2 and N_2O, the situation cannot be predicted in advance. However, calculations similar to those sketched above have been performed; then reliability depends on the accuracy of the input constants, but it is believed that such a computation is useful.

One must also note that in the isotopically modified molecules, the eigenvectors of resonating groups vary widely. Thus, the simple assumption of a constant isotopic abundance ratio for the intensities is very far from correct. It should be adequate however to assume that the relative intensities of the underlying transitions (301-0 and 221-0, in the example cited above) remain isotopically invarient.

It should also be remarked that the eigenvectors are rotationally dependent; the result would be a contribution to the m^2 term in Eq. (9).

4. MOLECULAR SPECIES

4.1 Water Vapor

4.1.1 LINE POSITIONS

The frequencies of the lines of the principal isotope ($^1H^{16}O^1H$ = Code 161) are calculated from a set of energy levels. These were obtained from the best available data in all spectral regions by a smoothing process which is partly theoretical, partly empirical. The principal sources of data are identified and summarized in Table 7. The energy levels of the ground state, $v_1v_2v_3$ = 000, are by far the most extensive and accurate. They are based on a relatively small number (15, at the present writing) of microwave lines whose frequencies are precise to < 0.00001 cm^{-1} (0.3 MHz), and several much larger groups of pure rotational lines, whose frequency accuracy may range from 0.001 to 0.002 cm^{-1} for isolated lines measured with Michelson-type interferometers to 0.02 to 0.03 cm^{-1} for weaker or partially blended lines measured with conventional spectrometers. With the long absorption paths available through the atmosphere, the observed lines extend to quite high energy levels, and by somewhat less accurate measurements with flame sources, to still higher levels, so that pure rotation transitions connect all levels from 0 to more than 4000 cm^{-1}. The 000 level is the lower state of the more than 50 vibration-rotation bands observed between 900 and 20,000 cm^{-1}, so that these measurements provide combination differences (common upper level in two or more transitions) for the 000 state that confirm, and for some states greatly improve those of the pure-rotation lines. In particular, the recent laboratory measurements of the 1.9 μm region give low-J energy differences that are self-consistent to better than 0.001 cm^{-1}. A theoretical smoothing of the totality of the observed microwave, pure-rotation, and combination-difference data, by least-squares fitting to a 29-constant Hamiltonian of the type described for D_2O (Benedict et al, 1970) then yields the ground state energy levels used in the compilation. Inasmuch as none of the theoretical calculations have been successful in reproducing all of the available data to their apparent accuracy, the levels adopted for the current compilation are a calculated set for $E < 2500$ cm^{-1}, and for higher energies are determined from observations. It is believed that the accuracy of lines involving these levels is $\pm$ 0.005 cm^{-1} for $E'' < 1500$ cm^{-1}; $\pm$ 0.02 cm^{-1} for $1500 < E'' < 3000$ cm^{-1}, and $\pm$ 0.05 cm^{-1} up to the tabulated limit. The levels of the other vibration-rotation states are then obtained by averaging the sums of the observed lines and the lower-state levels. When upper-state levels have not been observed, although transitions to them have expected intensities above the lower limit, estimated values are chosen, either by direct calculations using an appropriate approximate Hamiltonian, or by extrapolation of the observed series of upper-lower rotational energy differences.

For the isotopic forms 181 and 171, the ground-state energies were obtained in the same way, except with much less extensive data (respectively 12 and 9 microwave lines). The dependence on theoretical calculations for the smoothing is more extreme, and the data for levels higher than 1500 cm^{-1}, the limit of observation, is quite uncertain. However, since the higher-order constants in the

Table 7. Summary of Principal Data Sources for Water-Vapor Energy Levels

Region cm^{-1}	Type of Measurement	Range of Levels			Intensity Limit (296 K)	Precision of ν cm^{-1}	Ref.
		Vibrational	Rotational J	K_a			
0-25	L,181,171	0,010	10	6	<-27	.00001	a,b
0-25	L,162,182	0,010	13	7	<-27	.00001	c,d
30-250	L	0	13	7	-23	.005	e
250-550	L	0	15	11	-24	.03	f
480-690	LH	0	15	12	-25	.02	g
430-650	F	0,010 etc.	30	15	<-27	.05	h
700-1100	LH	0,010	19	12	-26	.1	i
750-1400	A	0,010	18	12	-25	.05	j
860-1100	A	0,010	18	12	-25	.02	k
1270-1450	LH	010,020	16	9	-27	.05	l
1200-1700	L,162	010	14	7	-27	.02	m
1330-1970	L,181,171	010	13	6	-26	.01	n
1840-2500	LH	010,020,001+	18	10	-26	.03	o,ℓ
1925-2182	A,U	010,020,001+	28	10	<-27	.01	p
2390-2970	A,U	100,001, etc.	32	19	<-27	.01	p
2480-3030	L,162	100,020	18	10	<-27	.005	q
2900-3500	A	020,100,001	16	11	-26	.02	r
2800-3500	F	001,011, etc.	33	13	<-27	.02	s
2900-4330	L,162	001,100, etc.	14	9	-25	.005	t *
3340-4030	L,181,171	001,100, etc.	13	7	-26	.01	u
3940-4300	F	001,011, etc.	33	19	<-27	.02	s
4032-5090	A,U	001,011,020 +	33	17	<-27	.01	v
3950-5200	A	001,030,011,etc	18	13	-26	.01	w
4500-5915	L,162	011,030,110,etc	14	8	-25	.005	t *
5090-5575	L	011,110	12	7	-24	.005	x
5540-7000	A	011,021,120 +	16	9	-26	.01	w
5550-6720	A,U	011,021,120 +	24	11	<-27	.01	v
7000-7500	L	101,200	13	8	-24	.05	y
7400-9000	A	101,002,111 +	16	9	-26	.01	w
7390-8800	A,U	101,001,111 +	16	9	-25	.01	v
8300-10000	A	111,012,041	16	8	-25	.03	z
9150-9350	A	012,111	10	7	-27	.005	aa

References:

a. DeLucia et al, 1972
b. Steenbeckeliers et al, 1971
c. De Lucia et al, 1971
d. Benedict et al, 1973
e. Hall and Dowling, 1967
f. Rao et al, 1962
g. Izatt et al, 1969
h. Madden and Benedict, 1956
i. Burch and Gryvnak, 1971
j. Dionne, 1972
k. Migeotte et al, 1957
l. Ben-Aryeh, 1967
m. Williamson et al, 1969
n. Gailar and Dickey, 1960
o. Burch and Gryvnak, 1973
p. Hall, 1972
q. Benedict et al, 1973
r. Beer, 1970
s. Benedict and Sams, 1971;
t. Pugh, 1972
u. Fraley et al, 1969
v. Hall, 1970
w. Connes et al, 1969
x. Flaud et al, 1972
y. Nelson, 1951
z. Swensson et al, 1970
aa. Breckenridge and Hall, 1973

Table 7. References for Water Vapor Energy Level Data (Contd)

The data sources are of five types: L, laboratory absorption measurements on water vapor or moist air at room temperature; LH, similar measurements in cells heated to 75-540°C; F, laboratory measurements of emission from oxy-hydrogen or oxy-acetylene flames, yielding ~10^{19} molecules/cm^2 H_2O at +2500-3500K; A, measurements of solar radiation through the atmosphere, containing 10^{22}-10^{25} molecules/cm^2; U, observations of the ratioed spectrum of sunspot/photosphere, also containing about 10^{19} mol/cm^2 at ~3600K. Isotopic symbols are appended when enriched samples were studied, underlined when a major component, dashed when moderately increased above natural abundance. The range of vibrational and rotational levels is a rough indication of the extent of levels observable down to the intensity limit of S^o (cm^{-1}/mol cm^{-2}), corrected to 296K, with the resolving power used. The ground state, (v=0) is implied in all regions.

* In reference t, the observed contamination of the sample by deuterium to give the HDO abundances varying from 10-200 times normal was not reported.

theoretical fit were constrained near their values in H_2O-161, the tabulated line positions for all pure-rotation lines should be accurate to ± 0.5 cm^{-1}. Upper-state levels for these molecules are likewise available only for the strongest lines, so that the uncertainties of weak lines here might approach ± 1 cm^{-1}.

The asymmetrically substituted HOD (162) molecule has been studied, both in the microwave and infrared regions with thoroughness comparable to 161, so that the frequency data, for the 000,010, 100, 020, 110, and 030 bands should be of the same accuracy as for 161. The 001 and 011 levels may have errors larger by a factor of five.

Quite reliable data can be calculated for the pure-rotation spectra of isotopic forms 182, 172, and 282, which are only of very minimal importance in the atmosphere. Weak lines in vibration-rotation bands of 182 (as yet unobserved, except for a few lines in 100-000) also have been included by estimating constant vibrational shifts from 162.

4.1.2 LINE INTENSITIES

The intensities of pure rotation lines were calculated by a program in which the effects of vibration-rotation interaction on both the rotational eigenfunctions and on the dipole moment were included. The eigenfunctions were obtained from a Hamiltonian with 25 independent constants which gave an excellent fit to the energy levels, and the dipole moment was expressed as a linear expansion in the dimensionless normal coordinates:

$$\mu = \mu_e + (\partial\mu/\partial q_1)q_1 + (\partial u/\partial q_2)q_2 + (\partial\mu/\partial q_3)q_3 + \ldots \qquad (14)$$

The $\partial\mu/\partial q_i$ coefficients in this expression were obtained from the S_v^o values of the three fundamental bands by the equation $S_{vi}^o = 4.16\times10^{-19}\,\nu(\partial\mu/\partial q_i)^2$. The algebraic signs of $\partial\mu/\partial q_i$ were chosen so that the observed vibration-rotation effects on intensities were reproduced in the fundamental bands of H_2O and verified by noting that these and only these choices also gave a reasonable fit to the band intensities and interaction effects in the isotopic molecules. The value of the permanent moment in the equilibrium configuration, μ_e = 1.847D (Clough and Beers, 1973), was derived from Stark Effect measurements on 8 microwave lines in three isotopic water molecules (161, 162, 262), and is in excellent agreement with recent molecular-beam measurements (Dyke and Muenter, 1972). The uncertainty in the calculated intensities should result from inaccuracy of the $\partial\mu/\partial q_i$ coefficients and neglect of higher terms in the expansion; accordingly, it should be of minor importance for low J lines, and is estimated to be less than 1 percent for $E'' < 1000$ cm^{-1} and less than 10 percent for all lines in the tabulation, with the possible exception of the very low probability lines in such branches as R_{53}, Q_{55}, etc. (Benedict, Classen and Shaw, 1952).

The intensities of vibration-rotation lines are more difficult to calculate, because they differ from those of the rigid asymmetric rotor by three interrelated effects: (1) the centrifugal effects, as used above for pure rotation; (2) the fact that the asymmetry, and hence the rotational eigenfunctions, are vibrationally dependent; and (3) the fact that for all vibrations above 010, the rotational levels of like symmetry and equal J in different vibrational levels are at energies sufficiently close that the vibrational eigenfunctions are rotationally dependent, and in special cases "perturbations" lead to abnormal mixing and intensities. Only the first-named effect has been incorporated in the computations, through the method described by Benedict and Calfee (1967). Table 8 lists the constants used for each band. The footnotes to Table 8 list the sub-branches which are observed to disagree in a regular way from the results of the calculation, and which were adjusted accordingly. The lines that are exceptionally perturbed (effect 3) are identified by the symbol P following K'_c; for these the total intensity of the two "interacting" lines was divided as required by the calculated vibrational mixing ratios or further adjusted to agree with measurements. No general statement can be made concerning the accuracy of the intensities of individual lines; for the low-J lines of the strongest bands it should be within ± 10 percent, within a factor of two for other lines of sufficient intensity ($> 10^{-25}$ cm^{-1}/mol-cm^{-2}) to appear in laboratory and/or solar spectra, and within an order of magnitude for the weakest lines.

The intensities of the isotopic lines of species 181 and 171 were taken equal to those of 161 multiplied by the abundance factor (except for the cases of strong perturbation where the vibrational mixing ratios are different). The asymmetric isotopic species 162 is widely different, so that a completely independent calculation of its intensities, in both pure rotation and vibration-rotation has been made. The band parameters are included in Table 8.

4.1.3 LINE WIDTHS

Recent high-resolution spectra of air-broadened or N_2-broadened water vapor lines (Brault, 1972, private communication) have in general confirmed the calculations of Benedict and Kaplan (1959) to ± 10 percent. A striking discrepancy is, however, observed (Blum et al, 1972) for the lines of highest J which are much narrower than the lower limit of 0.032 cm^{-1}atm^{-1} which was imposed on the calculated value by choosing a minimum collision diameter equal to the kinetic-theory diameter. If the Anderson Theory (Anderson, 1949) is modified by eliminating a distance of closest approach (that is, setting the kinetic theory collision diameter equal to zero) the calculated half-width at half-height of $16_{1,16}-15_{0,15}$ is lowered from 0.032 to 0.0098 cm^{-1}, still slightly above the observed value (0.0086). The validity of the theory is thus in question for high-J transitions but a revised

Table 8. Water Vapor Band Intensity Data and Interaction Coefficients

ν_0 cm^{-1}	iso	v' v"	Rot Type	S_v^0(296K) cm^{-1}/molcm^{-2}	R Debyes	Interaction Coefficients			
						α	β	γ	Notes
1403.489	162	010 000	A B	8.0 -022 1.92 -021	.066 .105				
1556.895	161	020 010	B	8.61 -021	.171				(1)
1588.279	181	010 000	B	2.12 -020	.121				(1)
1591.32	171	010 000	B	3.93 -021	.121				(1)
1594.736	161	010 000	B	1.061-017	.121	.025 .05	.0065 .013	-.004 -.005	(2)
2062.318	161	100 010	B	8.9 -023	.0167				
2161.188	161	001 010	A	4.9 -022	.0394		-.0108	-.015	
2709.35	182	100 000	A	1.31 -024	.0437				
2723.687	162	100 000	A B	6.53 -022 2.0 -023	.0437 .0076	.0322 -.1	.0130	.077	
2782.014	162	020 000	A B	8.1 -023 9.0 -024	.0153 .0051				
3072.058	161	030 010	B	7.99 -023	.0121				(1)
3139.02	181	020 000	B	1.32 -022	.0070				(1)
3144.96	171	020 000	B	4.92 -023	.0070				(1)
3151.631	161	020 000	B	6.58 -020	.0070		.005	.003	(3)
3640.245	161	110 010	B	1.50 -022	.0149				(1)
3649.690	181	100 000	B	7.24 -022	.0149				(1)
3653.14	171	100 000	B	1.33 -022	.0149				(1)
3657.054	161	100 00	B	3.62 -019	.0149	.075	.035	.028	(3)
3707.459	162	001 000	A B	1.2 -021 3.0 -022	.0509 .0255				
3736.509	161	011 010	A	3.30 -021	.0708				(1)
3741.571	181	001 000	A	1.60 -020	.0708				(1)
3748.36	171	001 000	A	2.96 -021	.0708				(1)
3755.924	161	001 000	A	7.994-018	.0708	.0695 .0278	.0310 .0124	.0160 .0064	(4)
4099.954	162	110 000	A B	2.0 -023 1.5 -024	.0088 .0024	(F=1+0.15Ka)			(5)
4145.483	162	030 000	A B	2.0 -023 1.5 -024	0	(F=1-0.15Ka-.05m)			(5)
4666.720	161	030 000	B	2.0 -022	.00032	.01	.10	.12	
5089.539	162	011 000	A B	3.0 -023 6.0 -024	.0069 .0031	.02			
5180.36	161	120 010	B	1.47 -023	.0040				(1)
5221.28	181	110 000	B	3.66 -023	.0028				(1)
5227.75	171	110 000	B	6.77 -024	.0028				(1)
5234.981	161	110 000	B	1.83 -020	.0028	.05	-.015	-.02	
5276.776	161	021 010	A	7.45 -022	.0286				(1)
5310.43	181	011 000	A	1.81 -021	.0203				(1)
5320.25	171	011 000	A	3.36 -022	.0203				(1)
5331.245	161	011 000	A	9.06 -019	.0203		.0144	.02	

Table 8. Water Vapor Band Intensity Data and Interaction Coefficients (Contd)

ν_0				S_v^0(296K)	R	Interaction Coefficients			
cm^{-1}	iso	v' v"	Rot Type	$cm^{-1}/mol\ cm^{-2}$	Ddbyes	α	β	γ	Notes
5372.114	162	200 000	A	1.2 -023	.0042				
6679.21	161	130 010	B	4.32 -024	.00194				
6755.40	181	120 000	B	7.05 -024	.00112				
6775.10	161	120 000	B	3.53 -021	.00112				
6779.08	161	031 010	A	6.94 -023	.0076				
6844.59	181	021 000	A	1.13 -022	.0044				
6857.32	171	021 000	A	2.09 -023	.0044				
6871.512	161	021 000	A	5.64 -020	.0044				
7186.68	181	200 000	B	1.06 -022	.0042				
7201.48	161	200 000	B	5.29 -020	.0042				
7213.26	161	111 010	A	3.98 -022	.0157				
7222.68	181	101 000	A	1.49 -021	.0157				
7235.57	171	101 000	A	2.76 -022	.0157				
7249.93	161	101 000	A	7.47 -019	.0157				
7371.79	161	012 010	B	2.17 -024	.00131				
7417.54	181	002 000	B	1.06 -023	.00131				
7430.54	171	002 000	B	1.96 -024	.00131				
7745.04	161	002 000	B	5.29 -021	.00131				
8238.84	161	041 010	A	5.88 -024	.00204				
8273.95	161	130 000	B	2.4 -022	.00027				
8341.32	181	031 000	A	7.2 -024	.00102				
8356.70	171	031 000	A	1.33 -024	.00102				
8373.82	161	031 000	A	3.6 -021	.00102				
8734.97	161	121 010	A	4.10 -023	.0037				
8761.57	161	210 000	B	3.6 -022	.00031				
8779.75	181	111 000	A	9.96 -023	.0037				
8792.63	171	111 000	A	1.85 -023	.0037				
8807.00	161	111 000	A	4.98 -020	.0037				
8966.53	181	012 000	B	2.4 -024	.00057				
9000.13	161	012 000	B	1.2 -021	.00057				
9833.58	161	041 000	A	4.8 -023	.00011				

Notes to Table 8.

(1) Insufficient data to establish interaction coefficients; these are assumed identical with corresponding band of 161.

(2) Lower line for strong lines (L rigid>1); upper line for others.

(3) Many lines, especially those with entranced resonance with 001, require special treatment.

(4) Lower line for strong lines (L rigid>0.5); upper line for others.

(5) Very close resonance of these two states at K_a=0, all transition moment attributed to 110-0.

calculation with $b_{min} = 0$ does reproduce the empirical results better than the original calculation. Accordingly this has been incorporated in the current tabulation. As in previous computations, no vibrational dependence of the width has been included. The widths of the isotopic lines (181 and 171) have been set equal to those of 161; for 162 a new calculation, with $\mu_e = 1.847$, $q_{air} = 2.62 \times 10^{-26}$ esu and $b_{min} = 0$ has been made, where μ_e is the dipole moment of water, q_{air} is the effective quadrupole moment of the colliding gas and b_{min} is the collision diameter.

4.2 Carbon Dioxide

4.2.1 LINE POSITIONS

The line positions and lower-state energies of each of the significant isotopic modifications of CO_2 were calculated for each band by a rotational formula for the linear molecule including terms up to $D_v J^2(J + 1)^2$. For some of the higher states involving Fermi resonances of high rank, an additional term $H_v J^3(J + 1)^3$ was required. A very few of the vibrational levels are involved in a rotational perturbation, for which special calculations were needed as discussed below. The constants for each level are summarized in Table 9. For each isotopic species the band constants form a self-consistent set; that is, if a vibrational state appears more than once, as either initial or final state, its value of G_v, B_v, D_v (and occasionally H_v) is the same. This requirement results in some deviations of the smoothed final line positions from their best observed values, but in general the positions of observed lines, up to $J = 40$, will be within $\pm$ 0.01 cm^{-1} of the tabulation.

The constants were calculated for each isotopic species separately, using a set of constants similar to those of Chedin and Cihla (1972), for 626, 636, and 628, but the isotopic sets were not consistently readjusted to fit a potential function. However, for isotopic forms for which the data are less extensive, approximate isotopic relations were used.

The data used for the band constants are taken from various sources. The highest precision data are those for the laser transitions 00011-10001 and 00011-10002 in the 626 isotope. The measurements of Gordon and McCubbin (1965, 1966), Oberly et al, (1968), and Drayson (1967) provide the data for interrelations among the lowest states. The most extensive data for the higher states are those from the planet Venus, as observed and summarized by Connes et al, (1969).

The vibrational notation may not be familiar to all users, and accordingly will be explained at this point. Five digits are used for each state, in order, $v_1 v_2 \ell v_3 r$. The fifth digit, r, takes the possible values 1, 2, . . . $v_1 + 1$, and serves to locate the level in the Fermi resonating group of $v + 1$ levels; v_1, v_2^{ℓ}, v_3; $v_1 - 1(v_2 + 2)^{\ell}, v_3$; . . . $0, (v_2 + 2v_1)^{\ell}, v_3$. The value of r decreases with increasing energy. (In

Table 9. Vibrational Energy Levels and Molecular Constants for CO_2

Energy Level	G (cm^{-1})	B (cm^{-1})	D Multiply by 10^{-7} (cm^{-1})
	Isotope 626		
00001	0.00	0.390218	1.331
01101 c	667.379	.390643	1.355
01101 d		.391253	1.355
10002	1285.412	.390481	1.563
02201 c	1335.129	.391682	1.389
02201 d			1.379
10001	1388.187	.390188	1.142
11102 c	1932.470	.390736	1.441
11102 d		.391680	1.501
03301 cd	2003.238	.392420	1.403
11101 c	2076.865	.390416	1.281
11101 d		.391344	1.195
00011	2349.146	.387140	1.325
20003	2548.280	.391183	1.76
12202 c	2585.006	.391843	1.45
12202 d			1.25
20002	2671.113	.389556	1.331
04401 cd	2671.690	.393162	1.42
12201 c	2760.735	.391535	1.44
12201 d			1.25
20001	2797.154	.390563	0.985
01111 c	3004.016	.387593	1.349
01111 d		.388190	1.349
21103 c	3181.450	.391028	1.63
21103 d		.392316	1.75
13302 cd	3240.564	.392696	1.51
21102 c	3339.340	.390035	1.37
21102 d		.391145	1.37
05501 cd	3340.475	.393908	1.44
13301 cd	3442.256	.392312	1.35
21101 c	3500.590	.390461	1.14
21101 d		.391700	1.01
10012	3612.844	.387496	1.57
02211 c	3659.277	.388647	1.383
02211 d			1.373
10011	3714.781	.387051	1.13
30004	3792.702	.391760	2.02
22203 c	3821.984	.392359	1.46
22203 d			1.68
14402 cd	3898.117	.393434	1.54
30003	3942.492	.389584	1.66
22202 c	4007.850	.391485	1.47
22202 d			1.40
30002	4063.908	.389606	0.935
14401	4122.347	.393036	1.36
22201 c	4197.413	.391719	1.63
22201 d			1.13
30001	4225.110	.391090	0.521
11112 c	4247.713	.387773	1.49
11112 d		.388690	1.56
03311 cd	4314.913	.389387	1.405
11111 c	4390.628	.387350	1.24
11111 d		.388230	1.17
00021	4673.327	.384063	1.319
31104 c	4416.150	.391357	1.63
31104 d		.393078	1.76
31103 c	4591.118	.389925	1.53
31103 d		.391348	1.48
33102 c	4753.450	.389708	1.20
31102 d		.391098	1.33
20013	4853.620	.388188	1.77
12212 c	4887.970	.388958	1.33
12212 d			1.43
31101 c	4938.410	.389358	0.995
31101 d		.391130	0.808
04411 cd	4970.909	.390148	1.42
20012	4977.830	.386529	1.35
12211 c	5061.776	.388508	1.28
12211 d			1.12
20011	5099.660	.387448	0.921
01121 c	5315.730	.384548	1.46
01121 d		.385148	1.46
40004	5197.249	0.390092	1.89
32203 c	5245.469	.391498	1.335
32203 d			1.535
21113 c	5475.071	.388153	1.61*
21113 d		.389123	1.705
40002	5475.565	.390093	0.895*
13312 cd	5531.279	.389732	1.52
05511 cd	5627.254	.390913	1.44
21112 c	5632.760	.387018	1.265
21112 d		.388128	1.385
13311 cd	5730.618	.389269	1.51
21111 c	5790.579	.387413	1.125
21111 d		.388613	1.025
10022	5915.209	.384528	1.57
02221 c	5958.539	.385617	1.35
02221 d			1.31
10021	6016.690	.383917	1.17
30014	6075.983	.386896	2.052
22213 c	6103.670	.389428	1.29
22213 d			1.67
14412 c	6176.623	.390485	1.54
41102 c	6179.010	.389642	1.33
30013	6227.924	.386697	1.643
22212 c	6288.492	.388472	1.38
22212 d			1.28
30012	6347.854	.386451	0.951
41101 c	6388.085	.390290	0.93
14411 cd	6398.047	.390017	1.37
22211 c	6474.530	.388662	1.53
22211 d			1.21
30011	6503.081	.387974	0.719
11122 c	6537.958	.384804	1.475
11122 d		.385722	1.606
11121 c	6679.709	.384310	1.216
11121 d		.385127	1.115
00031	6972.578	.380990	1.331
31114 c	6688.274	.388547	1.735
31114 d		.390246	1.825
31113 c	6863.553	.386930	1.401
31113 d		.388333	1.485
31112 c	7023.672	.386755	1.19
31112 d		.388127	1.165
20023	7133.819	.385288	1.75
12222 c	7166.049	.386017	1.15
12222 d			1.35
31111 c	7203.814	.387607	1.05
31111 d		.389117	0.85
12221 c	7338.149	.385487	1.33
12221 d			1.28
20021	7377.679	.384403	1.45
01131 c	7602.529	.381503	1.315
01131 d		.382063	1.355
40015	7283.981	.389550	2.31
32214 c	7307.651	.389942	1.03
32214 d			1.64
40014	7460.530	.387322	1.93
32213 c	7505.219	.388632	1.23
32213 d			1.34
40013	7593.690	.385562	1.04
32212 c	7694.416	.388252	1.18
32212 d			1.14
40012	7734.452	.386954	0.59
21123 c	7743.700	.385358	1.25
21123 d		.386488	1.73
32211 c	7897.573	.388965	1.33*
32211 d			0.939**
21122 c	7901.479	.384008	1.31*
21122 d		.385128	1.38**
40011	7920.840	.388558	0.60
21121 c	8056.024	.384408	1.11
21121 d		.385525	1.08
10032	8192.556	.381561	1.56
02231 c	8332.880	.382600	1.30
02231 d			1.28
10031	8293.957	.380805	1.13
41114 c	8081.179	0.387643	1.56
41114 d		.389753	1.66
41113 c	8250.644	.386233	1.355
41113 d		.387813	1.355
41112 c	8425.000	.386817	0.935
41112 d		.388517	0.965
11132 c	8803.265	.381858	1.49
11132 d		.382744	1.56
03331 cd	8863.548	.383420	1.40
11131 c	8944.146	.381264	1.22
11131 d		.381874	1.18
20033	9388.990	.38234	1.71
12232 c	9419.189	.38307	1.37
12232 d			1.25
20032	9516.970	.38048	1.39
12231 c	9589.929	.38247	1.43
12231 d			1.53
20031	9631.350	.38125	1.04
21133 c	9987.48	.38251	1.55
21133 d		.38351	1.63
21132 c	10145.43	.38096	1.25
21132 d		.38258	1.35
21131 c	10297.05	.38127	1.10
21131 d		.38237	1.00
	Isotope 636		
00001	0.00	.390235	1.330
01101 c	648.484	.390598	1.330
01101 d		.391236	1.330
10002	1265.820	.390920	1.58
02202 c	1297.269	.391603	1.274
02202 d			1.334
10001	1370.067	.389707	1.160
01102 c	1896.49	.391137	1.48
01102 d		.392096	1.13
03301 cd	1946.343	.392293	1.34
11101 c	2037.093	.390015	1.18
11101 d		.390975	1.13
00011	2283.490	.387300	1.325
20003	2507.50	.391815	1.76
12202 c	2531.63	.39220	1.22
12202 d			1.40
04401 cd	2595.614	.392987	1.34
20002	2645.086	.389826	1.46
12201 c	2700.25	.39126	1.30
12201 d			1.34
20001	2750.48	.389670	0.91
01111 c	2920.244	.387664	1.325
01111 d		.389286	1.325
21103 c	3127.28	.39155	1.70
21103 d		.39308	1.68
13302 cd	3169.21	.39272	1.45
21102 c	3289.71	.39001	1.25
21102 d		.39120	1.25
13301 cd	3361.57	.39188	1.25
21101 c	3433.70	.39292	1.04
21101 d			1.10
10012	3527.740	.388030	1.56
02211 c	3557.314	.388668	1.28
02211 d			1.33
10011	3632.917	.386726	1.21
30001	4145.95	.39010	1.22*
11112 c	4147.234	.38811	1.49*
11112 d		.38915	1.59
03311 cd	4194.704	.389348	1.33
11111 c	4287.695	.387654	1.27
11111 d		.387977	1.26
00021	4543.552	.384360	1.33
20013	4748.058	.388845	1.815
12212 c	4770.985	.38925	1.25
12212 d			1.27
04411 cd	4831.99	.39003	1.34

*,** J-dependent interactions

Table 9. Vibrational Energy Levels and Molecular Constants for CO_2 (Contd)

Energy Level	G (cm^{-1})	B (cm^{-1})	D Multiply by 10^{-7} (cm^{-1})
20012	4887.390	0.386847	1.47
12211 c	4938.80	.38831	1.44
12211 d			1.40
20011	4991.350	.386705	0.94
01121 c	5168.600	.384695	1.33
01121 d		.385305	1.33
21113 c	5357.004	.388614	1.50
21113 d		.390108	1.68
13312 cd	5397.09	.38978	1.30
21112 c	5519.944	.387038	1.16
21112 d		.388206	1.30
13311 cd	5588.17	.38907	1.44
21111 c	5662.269	.386837	1.10
21111 d		.387936	1.00
30014	5951.600	.389640	2.326
22213 c	5970.949	.389913	1.57
22213 d			1.33
30013	6119.618	.387540	1.786
22212 c	6155.37	.38852	1.36
22212 d			1.30
30012	6241.964	.385859	1.113
22211 c	6326.049	.388103	1.04
22211 d			1.35
30011	6363.616	.387033	0.906
11122 c	6374.497	.38521	1.46
11122 d		.38607	1.56
00031	6780.215	.381353	1.33
31114 c	6552.954	.388958	1.63
31114 d		.390896	1.83
31113 c	6736.694	.387368	1.63
31113 d		.388906	1.58
31112 c	6892.054	.386378	1.33
31112 d		.387706	1.18
31111 c	7046.029	.386858	1.23
31111 d		.388236	0.93
01131 c	7393.599	.381803	1.33
01131 d		.382391	1.33
40013	7481.510	.385435	0.33
40012	7600.130	.385855	0.63
10032	7981.180	.382275	1.52
10031	8089.040	.380735	1.26
	Isotope 628		
00001	0.00	.368164	1.11
01101 c	662.368	.368588	1.13
01101 d		.369128	1.13
10002	1259.430	.368114	1.26
02201 c	1325.15	.369520	1.20
02201 d			1.16
10001	1365.845	.368502	0.962
11102 c	1901.748	.36845	1.23
11102 d		.36925	1.28
03301 cd	1988.328	.370182	1.20
11101 c	2049.346	.36860	1.06
11101 d		.36954	1.01
00011	2332.112	.365267	1.11
20003	2500.776	.368463	1.44
12202 c	2549.425	.36954	1.25
12202 d			1.27
20002	2614.235	.367807	1.04
04401 cd	2651.875	.37085	1.22
12201 c	2728.264	.36966	1.30
12201 d			1.07
20001	2757.229	.369039	0.77
01111 c	2982.106	.365707	1.13
21103 c	3127.31	.36855	1.34
21103 d		.36957	1.43
13302 cd	3200.15	.37023	1.28
21102 c	3281.07	.36817	1.14

Energy Level	G (cm^{-1})	B (cm^{-1})	D Multiply by 10^{-7} (cm^{-1})
21102 d	3281.07	0.36916	1.12
13301 cd	3404.93	.37077	1.28
21101 c	3453.99	.36881	0.98
21101 d		.37007	0.90
10012	3571.143	.365284	1.27
02211 c	3632.52	.366595	1.19
d			1.15
10011	3675.130	.365524	0.95
30003	3856.657	.367405	1.24
30002	3987.610	.368174	0.91
11112 c	4201.19	.365666	1.23
11112 d		.366423	1.28
03311 cd	4283.35	.36726	1.19
11111 c	4346.13	.365716	1.05
11111 d		.366568	1.00
00021	4639.502	.362372	1.11
20013	4791.260	.365734	1.50
12212 c	4836.63	.366707	1.25
d			1.27
20012	4904.850	.364844	1.11
12211 c	5012.55	.366735	1.26
d			1.06
20011	5042.570	.366124	0.86
01121 c	5277.147	.362848	1.06
d		.363356	1.06
21113 c	5406.068	.365893	1.41
d		.366904	1.31
21112 c	5558.553	.365318	1.10
d		.366240	1.10
21111 c	5727.048	.365948	1.11
d		.367138	0.81
10022	5858.022	.362490	1.357
02221 c	5915.23	.36376	1.18
d			1.15
10021	5959.594	.362605	0.896
30014	5993.581	.366337	1.78
30013	6127.782	.364495	1.31
30012	6254.592	.365274	0.80
30011	6429.172	.366616	0.60
00031	6922.210	.359479	1.10
10032	8120.104	.359684	1.25
10031	8220.363	.359656	0.95
	Isotope 627		
00001	0.00	.378641	1.205
01101 c	664.735	.379065	1.22
01101 d		.379639	1.22
10002	1271.875	.378738	1.40
02201 c	1329.87	.380061	1.24
02201 d			1.22
10001	1376.28	.378806	1.04
11102 c	1916.31	.37903	1.27
11102 d		.37989	1.32
03301 cd	1995.36	.37977	1.22
11101 c	2052.41	.37894	1.15
11101 d		.37987	1.10
00011	2340.01	.375659	1.20
20003	2523.58	.37924	1.60
12202 c	2566.33	.380125	1.35
12202 d			1.25
20002	2641.26	.37814	1.18
12201 c	2743.68	.38005	1.20
12201 d			1.23
20001	2776.00	.37927	0.88
01111 c	2992.310	.376103	1.22
01111 d		.376664	1.22
10012	3590.86	.375835	1.38
02211 c	3645.02	.377091	1.24
02211 d			1.22
10011	3693.64	.375754	1.06

Energy Level	G (cm^{-1})	B (cm^{-1})	D Multiply by 10^{-7} (cm^{-1})
11112	4223.33	0.37616	1.31
11112 d		.37700	1.34
11111 c	4367.08	.37600	1.18
11111 d		.37686	1.15
00021	4655.205	.372674	1.20
20013	4821.500	.376411	1.62
20012	4939.350	.375131	1.21
20011	5064.910	.376321	1.00
21112 c	5593.645	.375625	1.22
21112 d		.376759	1.22
00031	6945.610	.369691	1.20
	Isotope 638		
00001	0.00	.368180	1.11
01101 c	643.23	.36857	1.12
01101 d		.36912	1.12
10002	1244.93	.36820	1.30
02201 c	1286.86	.36951	1.14
02201 d			1.11
10001	1342.37	.36844	0.90
00011	2265.973	.365388	1.11
20002 c	2588.43	.36778	1.04
01111 c	2897.58	.36579	1.12
01111 d		.36633	1.12
10012	3490.39	.36588	1.26
02211 c	3529.59	.36671	1.14
02211 d			1.12
10011	3587.54	.36525	1.01
00021	4508.749	.36260	1.11
20012	4814.570	.364810	1.11
	Isotope 637		
00001	0.00	.378658	1.21
01101 c	645.72	.379036	1.22
01101 d		.379627	1.22
10002	1254.83	.37900	1.40
02201 c	1292.80	.38000	1.22
02201 d			1.22
10001	1355.52	.37849	1.04
00011	2274.33	.37579	1.21
01111 c	2918.38	.37617	1.22
01111 d		.37675	1.22
10002	3508.07	.37641	1.41
10001	3609.05	.37540	1.11
	Isotope 828		
00001	0.00	.346799	1.04
01101 c	657.33	.347224	1.04
01101 d		.347736	1.04
10002	1230.20	.34620	
02201 c	1315.08	.34812	1.10
02201 d			1.04
10001	1347.22	.34776	
00011	2313.97	.34412	1.04
01111 c	2959.06	.34455	1.04
01111 d		.34504	1.04
10002	3525.205	.343840	1.16
10001	3638.067	.344636	0.907
	Isotope 728		
00001	0.00	.35695	1.07
01101 c	659.70	.35737	1.08
01101 d		.35789	1.08
00011	2322.52	.35419	1.07

this scheme, v_2 is always equal to ℓ.) The desirability of labelling the states in Fermi resonance by the same symbols except for r is to emphasize the very important role played by the Fermi resonance, which is very nearly exact for most of the groups. It must also be emphasized very strongly that the long-established custom of calling the upper level of the $(10^00, 02^00)$ resonance at 1388.18 cm^{-1}, ν_1, and the lower level at 1285.41, $2\nu_2$, is not only confusing the issue, but is wrong, since the now ten year old work of Amat and Pindert (1965) has shown that the unperturbed position of $2\nu_2^o$ lies above that of $\nu^o{}_1$, in the 626 isotope. This is also true in 627, 628, and 828, but in 636, 637, 638, it lies below. It seems vastly preferable always to label the upper level 10001 and the lower 10002.

4.2.2 LINE INTENSITIES

The intensity data (summarized in Table 10) are based on quantitative studies of resolved lines where such exist; and where not, on total intensities in a given region. The relations between the strengths of the principal band in a region and its associated weaker "hot" and isotopic neighbors were based on computations relating the transition moments to the vibrational eigenfunctions, taking into account terms up to the quartic in the molecular constants, with particular attention to the degree of Fermi mixing in the states, and an approximate calculation of the "unperturbed" (before Fermi mixing) transition moments. This procedure appears to give fairly good agreement for the ground-state and "first-hot" transitions in such Fermi groups as 2001-0000 and 3001-0000, and seems adequate for estimating strengths of higher unobserved hot bands. However, when experimental data are available (Burch, 1970), as for the 12201-11102 band at 828.28 cm^{-1}, these were used.

For the isotopic molecules, empirical data were again used where available, as for 628 bands which are forbidden in the symmetric molecules. When the isotopic bands overlap stronger bands of 626, the abundance ratios were used to estimate the total strength of a group, but the particular Fermi parameters were used to divide the strengths.

The influences of vibration-rotation interactions on line intensities has been measured in some cases. As a generalization, it can be said that these are usually negligible for the parallel bands ($\ell' - \ell'' = 0$) but become of considerable importance for all the perpendicular bands ($\ell' - \ell'' = \pm 1$) except those in the 15 μm region. For all the other bands, Coriolis-type resonances are responsible for inducing a large part of the transition moment in the R- and P-branches, thus "borrowing" intensity from the stronger parallel bands, while leaving the Q-branches unchanged. Accordingly, the latter may remain very weak (or in some cases be unobservable - for example, the 410 group). We have used the approximate equation $S_m = S^o{}_v (1 + m \zeta_v)^2$ to correct for this interaction, with the values

Table 10. Band Origins and Intensities for CO_2

Band Center ν_o (cm^{-1})	Upper Level	Lower Level	Isotope	S_v^o at 296K (multiply by 10^{-22} mol^{-1} cm^2 cm^{-1})	j
471.415	20003	11101	626	0.0087	
479.829	13302	12201	626	.0012	
494.537	12202	11101	636	.00079	Q
508.141	12202	11101	626	.0516	
510.337	21103	20002	626	.0040	
526.423	11102	10001	636	.035	
535.903	11102	10001	628	.0011	Q
542.186	21102	20001	626	.00711	
544.283	11102	10001	626	2.723	
548.275	13302	04401	628	0.00026	Q
557.742	14402	05501	626	.00253	
561.097	12202	03301	628	.0058	
564.889	20002	11101	628	.0043	
568.874	13302	04401	626	.0716	
570.87	12202	03301	627	.00092	Q
573.536	13302	04401	636	.00115	
576.598	11102	02201	628	.169	
578.605	21102	12201	626	.0376	
578.85	20002	11101	627	.00072	Q
580.424	22203	13302	626	.0096	
581.768	12202	03301	626	1.934	
585.287	12202	03301	636	.034	
586.44	11102	02201	627	.0439	
589.46	21102	12201	636	.00055	Q
594.248	20002	11101	626	.908	
595.65	21103	12202	636	.0038	
596.444	21103	12202	626	.257	
597.062	10002	01101	628	5.19	
597.341	11102	02201	626	52.08	
599.028	20003	11102	628	0.021	
599.221	11102	02201	636	.702	
601.70	10002	01101	638	.055	
607.14	10002	01101	627	1.17	
607.27	20003	11102	628	0.021	
607.993	20002	11101	636	.0111	
608.828	10012	01111	626	.0175	
609.11	10002	01111	637	.0106	
611.01	20003	11102	636	.102	
615.810	20003	11102	626	6.89	
617.336	10002	01101	636	20.5	
618.033	10002	01101	626	1436.	
619.78	21103	20003	636	0.0085	
633.170	21103	20003	626	.649	
636.754	01111	00011	636	.0121	
637.58	13302	12202	636	.013	
640.670	11102	10002	636	2.60	
642.318	11102	10002	628	0.78	
643.23	01101	00001	638	3.57	
644.435	11102	10002	627	0.15	
645.72	01101	00001	637	.642	
646.11	02201	01101	637	.055	
647.058	11102	10002	626	.222	
648.484	01101	00001	636	860.	
648.785	02201	01101	636	73.4	
649.074	03301	02201	636	4.69	
649.331	04401	03301	636	0.266	
649.580	05501	04401	636	.0142	
650.02	12202	11102	627	.0118	
652.536	12202	11102	626	16.52	
654.870	01111	00011	626	0.885	
655.558	13302	12202	626	0.990	
657.33	01101	00001	828	.343	
657.69	02202	00111	828	.0277	
657.553	14402	13302	626	.0442	
659.79	01101	00001	728	.0635	
661.32	13301	12201	636	.0055	
662.368	01101	00001	628	330.	
662.782	02201	01101	628	26.2	
663.157	12201	11101	636	0.106	
663.178	03301	02201	628	1.50	
663.547	04401	03301	628	0.078	
664.735	01101	00001	627	62.2	
665.135	02201	01101	627	4.88	
665.49	03301	02201	627	0.285	
667.026	11101	10001	636	1.58	
667.379	01101	00001	626	82580.	
667.750	02201	01101	626	6488.	
668.109	03301	02201	626	382.4	
668.227	21102	20002	626	0.312	
668.452	04401	03301	626	18.45	
668.785	05501	04401	626	0.976	
669.106	06601	05501	626	.077	
678.918	12201	11101	628	.060	
681.27	12201	11101	627	.0082	Q
681.521	13301	12201	626	.460	
683.501	11101	10001	628	.77	
683.870	12201	11101	626	9.05	
686.13	11101	10001	627	0.13	
688.678	11101	10001	626	148.8	
696.823	22201	21101	626	0.0195	
699.14	10001	01101	638	.058	
703.477	10001	01101	628	8.20	
703.436	21101	20001	626	0.246	
707.883	20001	11101	628	.024	
709.80	10001	01101	637	.0094	
710.765	10011	01111	626	.0202	
711.455	10001	01101	627	1.26	
712.487	20002	11102	628	0.013	
713.387	20001	11101	636	.047	
713.59	20001	11101	627	.0038	
720.289	20001	11101	626	4.784	
720.808	10001	01101	626	1853.	
721.583	10001	01101	636	17.9	
724.196	11101	02201	628	0.315	
724.95	20002	11102	627	.0024	Q
732.54	11101	02201	627	.0474	
733.45	21101	20001	636	.0021	Q
738.643	20002	11102	626	3.021	
739.824	11101	02201	636	0.70	
739.936	12201	03301	628	.0157	
739.855	21101	12201	626	.176	
741.736	11101	02201	626	79.01	
747.32	12201	03301	627	0.0025	Q
748.546	20002	11102	636	.0378	
753.055	13301	04401	628	.00058	Q
754.334	21102	12202	626	.1607	
757.497	12201	03301	626	3.288	
765.896	13301	04401	636	0.00173	Q
770.355	13301	04401	626	.1351	
771.273	11101	10002	636	.138	
781.872	14401	05501	626	.0051	
789.916	11101	10002	628	.0056	
790.536	11101	10002	627	.0010	Q
791.060	21102	20003	626	.0548	
791.452	11101	10002	626	11.23	
803.76	12201	11102	636	0.0052	
826.516	12201	11102	628	.0009	Q
828.265	12201	11102	626	.201	
829.467	21101	20003	626	.0548	
857.250	13301	12202	626	.0110	
864.684	20001	11102	626	.0432	
883.151	01111	11101	636	.00495	
898.542	02211	12201	626	.0132	
913.423	00011	10001	636	.0614	
915.584	21101	12202	626	.00195	Q
917.627	10011	20001	626	.0087	
927.151	01111	11101	626	.3556	
932.760	01111	11101	628	.00135	
941.731	10012	20002	626	.01146	
952.310	21101	20003	626	.00064	Q
960.959	00011	10001	626	4.910	
963.73	00011	10001	627	.0032	
966.267	00011	10001	628	.0195	
1017.670	00011	10002	636	.0726	
1023.744	01111	11102	636	.00072	
1063.734	00011	10002	626	6.324	
1068.135	00011	10002	627	.0047	
1071.546	01111	11102	626	.540	
1072.682	00011	10002	628	.0285	
1074.271	02211	12202	626	.0227	
1080.358	01111	11102	628	.00243	
1239.380	11102	01101	628	0.0351	
1244.93	10002	00001	638	.0038	
1259.430	10002	00001	628	.382	
1271.875	10002	00001	627	.0220	
1342.37	10001	00001	638	.0068	
1365.845	10001	00001	628	.561	
1376.28	10001	00001	627	.0323	
1386.978	11101	01101	628	.0516	
1846.321	21101	02201	626	.00033	-.15
1859.02	20003	01101	636	.00016	-.15
1860.232	30004	11102	626	.00002	-.12
1865.607	30003	11101	626	.00007	-.12
1880.901	20003	01101	626	.0156	-.20

Table 10. Band Origins and Intensities for CO_2 (Contd)

Band Center ν_o (cm^{-1})	Upper Level	Lower Level	Iso-tope	S_V^0 at 296K (multiply by 10^{-22} mol^{-1} cm^2 cm^{-1})	ζ
1883.146	12202	01101	636	0.00149	-.06
1889.514	22203	11102	626	.00127	-.08
1896.490	11102	00001	636	.0149	-.06
1896.038	21103	10002	626	.01101	-.07
1901.748	11102	00001	628	.02976	-.06
1905.435	13302	02201	626	.1786	-.06
1917.627	12202	01101	626	.4226	-.055
1930.985	22202	11101	626	.00082	-.06
1932.470	11102	00001	626	4.092	-.062
1951.153	21102	10001	626	.00707	-.06
1997.602	20002	01101	636	.0015	-.04
2003.734	20002	01101	626	.00818	-.03
2004.211	21102	02201	626	.00118	-.04
2010.022	30003	11102	626	.00013	-.05
2037.093	11101	00001	636	.186	-.05
2049.346	11101	00001	628	.0372	-.03
2055.846	12201	01101	628	.0052	-.03
2062.41	11101	00001	627	.0052	-.035
2075.380	22202	11102	626	.0085	-.04
2076.865	11101	00001	626	22.32	-.041
2093.356	12201	01101	626	3.958	-.038
2094.861	20001	01101	628	0.0055	-.04
2101.996	20001	01101	636	.0149	-.03
2107.127	13301	02201	626	.253	-.035
2112.461	21101	10001	626	.112	-.08
2119.119	14401	03301	626	.0156	-.033
2120.548	22201	11101	626	.0119	-.04
2127.235	12212	12201	626	.00247	
2129.775	20001	01101	626	1.302	-. 2
2148.245	30001	11101	626	.00595	-.10
2157.673	10012	10001	636	.0152	
2165.461	21101	02201	626	.0595	-.05
2170.848	11112	11101	626	.0507	
2180.676	20012	20001	626	.00092	
2182.507	20013	20002	626	.00172	
2205.298	10012	10001	628	.00558	
2224.647	10012	10001	626	1.272	
2225.05	05511	05500	636	0.00261	
2227.88	13312	13302	636	.00401	
2229.724	21113	21103	636	.00488	
2230.234	21112	21102	636	.00216	
2236.696	04411	04401	636	.0632	
2238.55	12211	12201	636	.0384	
2239.355	12212	12202	636	.129	
2240.558	20013	20003	636	.0724	
2240.87	20011	20001	636	.0122	
2242.696	20012	20002	636	.0258	
2242.776	00021	00011	638	.00124	
2242.73	02211	02201	638	.149	
2245.17	10011	10001	638	.0555	
2245.46	10012	10002	638	.0816	
2248.356	01121	01111	636	.0280	
2248.361	03311	03301	636	1.52	
2250.607	11111	11101	636	0.96	
2250.7[illegible]4	11112	11102	636	1.91	
2251.01	02211	02201	637	0.0264	
2253.24	10012	10002	637	0.0146	
2253.53	10011	10001	637	.0098	
2254.35	01111	01101	638	3.48	
2260.045	02211	02201	636	34.6	
2260.062	00021	00011	636	0.306	
2261.920	10012	10002	636	20.3	
2262.66	01111	01101	637	0.628	
2262.850	10011	10001	636	12.3	
2265.973	00011	00001	628	38.8	
2271.763	01111	01101	636	818.	
2274.33	00011	00001	637	7.15	
2274.367	06611	06601	626	0.0068	
2281.688	22213	22203	626	.0389	
2282.69	04411	04401	628	.0157	
2283.490	00011	00001	636	9602.	
2284.286	12211	12201	628	0.0115	
2286.779	05511	05501	626	.1942	
2287.205	12212	12202	628	.0262	
2288.152	13311	13301	626	.1183	
2290.615	20012	20002	628	.0107	
2290.484	20013	20003	628	.0180	
2290.715	13312	13302	626	.3125	
2293.420	21112	21102	626	.1919	
229[illegible].621	21113	21103	626	.3965	
2296.784	11111	11101	628	.325	
2295.022	03311	03301	628	.406	
2299.219	04411	04401	626	4.895	
2299.262	02221	02211	626	0.076	
2299.442	11112	11102	628	0.686	
2301.041	12211	12201	626	3.17	
2301.73	01111	01101	828	0.31	
2301.909	10021	10011	626	0.0289	
2302.365	10022	10012	626	0.0473	
2305.340	20013	20003	626	4.352	
2306.717	20012	20002	626	2.396	
2307.02	11112	11102	627	0.116	
2307.37	02211	02201	628	10.5	
2307.39	00021	00011	628	0.0791	
2309.285	10011	10001	628	4.47	
2311.675	03311	03301	626	122.8	
2311.713	10012	10002	628	7.29	
2311.715	01121	01111	626	1.793	
2313.764	11111	11101	626	8.56	
2313.97	00011	00001	828	3.60	
2315.15	02212	02202	627	1.91	
2315.243	11112	11102	626	17.11	
2317.36	10011	10001	627	0.805	
2318.985	10012	10002	627	1.29	
2319.738	01111	01101	628	258.	
2322.52	00011	00001	728	1.35	
2324.148	02211	02201	626	3080.	
2324.182	00021	00011	626	20.98	
2326.594	10011	10001	626	1183.	
2327.432	10002	10002	626	1934.	
2327.575	01111	01101	627	49.7	
2332.112	00011	00001	628	3330.	
2336.637	01111	01101	626	76600.	
2340.01	00011	00001	627	637.	
2349.146	00011	00001	626	959800.	
2367.097	10011	10002	636	0.0131	
2415.700	10011	10002	628	.0056	
2428.547	20011	20002	626	.00146	
2429.369	10011	10002	626	1.059	
2429.550	20012	20003	626	0.00256	
2458.158	11111	11102	626	.0402	
2464.942	21103	01101	628	.0058	
2500.776	20003	00001	628	.075	
2523.58	20003	00001	627	.0060	
2588.43	20003	00001	638	.0020	
2614.235	20002	00001	628	.186	
2618.702	21102	01101	628	.0148	
2641.26	20002	00001	627	.018	
2757.229	20001	00001	628	.022	
2776.00	20001	00001	627	.0023	
2791.622	21101	01101	628	.0015	
3125.323	30004	01101	626	.00024	.40
3154.605	22203	01101	626	.00074	.40
3181.45	21103	00001	626	.00687	.30
3275.113	30003	01101	626	.0102	.02
3281.07	21102	00001	628	.00017	.14
3289.71	21102	00001	636	.00042	.14
3339.340	21102	00001	626	.0417	.14
3340.471	22202	01101	626	.0063	.14
3396.529	30002	01101	626	.00185	.30
3398.206	21113	11101	626	.00413	
3450.75	13311	03301	636	.0174	
3460.514	21113	11102	636	.0409	
3465.433	20013	10001	626	.1786	
3473.716	12212	02201	636	.3422	
3482.238	20013	10002	636	.450	
3482.851	21112	11101	636	.0134	
3490.390	10012	00001	638	.463	
3497.464	30001	01101	636	.0 pert	
3498.750	11112	01101	636	7.314	
3500.590	21101	00001	626	.1052	.14
3504.320	21101	11102	628	.0110	
3504.933	14412	04401	626	.0475	
3508.07	10012	00001	637	.0771	
3509.207	21102	11101	628	.00462	
3511.58	11112	01101	628	.181	
3517.323	20012	10001	636	.177	
3525.205	10012	00001	828	.0588	
3527.703	30014	20003	626	.1034	
3527.740	10012	00001	636	94.2	
3527.757	22212	12201	626	.0374	
3531.83	20013	10002	628	.181	
3533.942	11122	01111	626	.0353	
3538.822	11112	01101	628	4.449	
3539.005	20012	10001	628	.0762	
3542.601	21113	11102	626	3.147	
3543.095	40002	11102	626	.0 pert	

Table 10. Band Origins and Intensities for CO_2 (Contd)

Band Center ν_o (cm^{-1})	Upper Level	Lower Level	Iso-tope	S_v^o at 296K (multiply by 10^{-22} mol^{-1} cm^2 cm^{-1})	ζ
3549.625	20013	10002	627	0.0224	
3550.700	30012	20001	626	0.0195	
3552.841	12212	02201	626	31.25	
3555.895	21112	11101	626	1.101	
3556.749	30013	20002	626	0.0629	
3558.595	11112	01101	627	.668	
3563.070	20012	10001	627	.0135	
3566.063	10022	00011	626	.208	
3568.208	20013	10002	626	33.78	
3571.143	10012	00001	628	52.2	
3578.670	22213	12202	626	0.138	
3580.334	11112	01101	626	803.5	
3587.540	10011	00001	638	0.703	
3590.86	10012	00001	627	8.41	
3609.05	10011	00001	637	0.126	
3612.844	10012	00001	626	10350.	
3621.283	20011	10001	636	0.283	
3621.570	20012	10002	636	0.435	
3623.454	21112	11102	636	.0433	
3625.176	21111	11101	636	.0324	
3632.917	10011	00001	636	160.	
3638.067	10021	00001	828	0.0392	
3641.717	13311	03301	636	.0240	
3659.277	02211	00001	626	(1.7-06 Δ)	
3655.42	20012	10002	628	.187	
3656.805	21112	11102	628	.0149	
3667.475	20012	10002	627	.0333	
3667.544	10021	00011	626	.383	
3675.130	10011	00001	628	47.8	
3675.694	11121	01111	626	0.0331	
3676.725	20011	10001	628	.164	
3676.741	30012	20002	626	.0915	
3679.644	30013	20003	626	.0986	
3683.762	11111	01101	628	3.884	
3687.702	21111	01111	628	0.0134	
3687.40	12211	02201	628	.143	
3692.418	20012	10002	626	'2.4	
3693.640	10011	00001	627	10.2	
3699.064	20011	10001	627	0.0279	
3700.290	21112	11102	626	3.549	
3702.345	11111	01101	627	0.771	
3703.486	22212	12202	626	.1503	
3705.927	30011	20001	626	.0551	
3711.473	20011	10001	626	35.01	
3713.714	21111	11101	626	2.816	
3713.795	22211	12201	626	0.1094	
3714.781	10011	00001	626	15000.	
3723.249	11111	01101	626	1135.	
3725.530	20011	10002	636	0.0078	
3726.351	14411	04401	626	.0499	
3726.647	12211	02201	626	48.5	
3727.380	13311	03301	626	2.09	
3783.14	20011	10002	628	0.0035	
3799.574	30012	20003	626	.0028	
3814.248	20011	10002	626	0.770	
3831.968	30011	20002	626	.00092	
3858.109	21111	11102	626	.0251	
3856.657	30003	00001	628	.016	
3987.610	30002	00001	628	.0149	
4005.948	00021	01101	626	.00818	.14
4416.150	31104	00001	626	.00037	.15
4508.749	00021	00001	638	.00186	
4529.870	40004	01101	626	.00023	.12
4578.090	32203	01101	626	.00018	.20
4591.118	31103	00001	626	.00205	.18
4614.779	01121	01101	628	.01042	
4639.502	00021	00001	628	.1302	
4655.205	00021	00001	627	.0127	
4671.680	22213	02201	636	.00149	
4685.780	30014	10002	636	.00186	
4687.796	30014	10001	626	.00521	
4692.180	20013	00001	638	.00260	
4708.52	21113	01101	636	.0298	
4733.50	23313	03301	626	.00670	
4743.70	21113	01101	628	.0335	
4748.058	20013	00001	636	.214	
4753.450	31102	00001	626	.00298	.10
4755.705	31114	11102	626	.0179	
4768.541	22213	02201	626	.2604	
4784.675	20023	00011	626	.00149	
4786.688	31113	11101	626	.0119	
4790.571	30014	10002	626	.1562	
4791.260	20013	00001	628	.469	
4807.692	21113	01101	626	6.695	
4808.188	40002	01101	626	0. pert	
4814.570	20012	00001	638	.0134	
4821.500	20013	00001	627	.0744	
4839.737	30013	10001	626	.1376	
4853.620	20013	00001	626	80.7	
4871.46	21112	01101	636	.238	
4887.390	20012	00001	636	2.976	
4887.970	12212	00001	626	(8.1-08 Δ)	
4896.185	21112	01101	628	.0893	
4904.850	20012	00001	628	1.116	
4925.010	20011	00001	638	0.00446	
4928.910	21112	01101	627	.00744	
4931.083	3113	11102	626	.0967	
4939.350	20012	00001	627	.2306	
4942.512	30013	10002	626	1.414	
4946.807	31112	11101	626	0.0595	
4953.363	22212	02201	626	1.042	
4959.667	30012	10001	626	0.837	
4965.381	21112	01101	626	26.56	
4977.830	20012	00001	626	349.7	
4991.35	20001	00001	636	2.12	
5013.785	21101	01101	636	0.1711	
5028.78	22211	02201	636	.00298	
5042.57	20011	00001	628	.227	
5061.776	12211	00001	626	(9.2-08 Δ)	
5062.442	30012	10002	626	.238	
5064.680	21111	01101	628	.260	
5068.910	20011	00001	627	.0632	
5099.66	20011	00001	626	112.3	
5114.894	30011	10001	626	0.309	
5123.20	21111	01101	626	10.64	
5139.401	22211	02201	626	0.409	
5168.60	01121	00001	636	.00372	
5217.669	30001	10002	626	.0234	
5247.030	10022	01101	626	.0101	
5277.07	01121	00001	628	.00149	
5291.16	02221	01101	626	.0275	
5315.73	01121	00001	626	.398	
5349.36	10021	01101	626	.00506	
5584.391	00031	10001	626	.00707	
5687.166	00031	10002	626	.00751	
5858.022	10022	00001	628	.00372	
5951.600	30014	00001	636	.00179	
5959.954	10021	00001	628	.00335	
5972.52	32214	02201	626	.00253	
5993.581	30014	00001	628	.00357	
6020.795	31114	01101	626	.0465	
6072.343	40014	10001	626	.00104	
6075.983	30014	00001	626	.454	
6088.21	31113	01101	636	.00238	
6100.30	31113	01101	628	.00208	
6119.618	30013	00001	636	.0290	
6127.782	30013	00001	628	.0238	
6149.760	41114	11102	626	.00179	
6170.090	32213	02201	626	.01265	
6175.118	40014	10002	626	.02269	
6175.950	30013	00001	627	.00320	
6179.01	41102	00001	626	(1.5-06 π)	
6196.174	31113	01101	626	.268	
6205.503	40013	10001	626	.0127	
6227.924	30013	00001	626	4.27	
6241.964	30012	00001	636	.0461	
6243.57	31112	01101	636	.00409	
6254.592	30012	00001	628	.01414	
6265.170	31112	01101	628	.00119	
6298.110	30012	00001	627	.00275	
6308.278	40013	10002	626	.02455	
6318.17	41113	11102	626	.00179	
6346.265	40012	10001	626	.0119	
6347.854	30012	00001	626	4.27	
6356.293	31112	01101	626	0.327	
6359.287	32212	02201	626	.0116	
6363.616	30011	00001	636	.0127	
6388.015	41101	00001	626	(4.8-06 π)	
6397.545	31111	01101	636	.00119	
6429.172	30011	00001	628	.00112	
6466.440	20023	01101	626	.00104	
6498.67	12222	01101	626	.00119	
6503.081	30011	00001	626	.498	
6532.653	40011	10001	626	.00130	

Table 10. Band Origins and Intensities for CO_2 (Contd)

Band Center ν_o (cm^{-1})	Upper. Level	Lower Level	Iso- tope	S_ν^o at 296K (multiply by 10^{-22} mol^{-1} cm^2 cm^{-1})	γ
6536.445	31111	01101	626	.0476	
6537.958	11122	00001	626	.0223	
6562.444	32211	02201	626	.00223	
6679.709	11121	00001	626	.0283	
6745.115	01131	01101	636	.01339	
6780.215	00031	00001	636	.1637	
6860.410	03331	03301	626	.00201	
6867.280	11131	11101	626	.00112	
6870.796	11132	11102	626	.00241	
6885.150	01131	01101	628	.00402	
6897.751	02231	02201	626	.0424	
6905.770	10031	10001	626	.0171	
6907.144	10032	10002	626	.0290	
6922.210	00031	00001	628	.0521	
6935.150	01131	01101	626	1.131	
6945.610	00031	00001	627	0.0112	
6972.578	00031	00001	626	14.95	
7283.981	40015	00001	626	0.00186	
7460.530	40014	00001	626	.0428	
7481.51	40013	00001	636	.00112	
7583.265	41113	01101	626	.00833	
7593.690	40013	00001	626	.1064	
7616.620	51102	00001	626	(1.12-06 π)	
7734.452	40012	00001	626	.0279	
7757.621	41112	01101	626	.00298	
7901.479	21122	00001	626	.00149	.018
7920.840	40001	00001	626	.00186	
7981.180	10032	00001	636	.00232	
8084.060	12232	02201	626	.00193	
8089.84	10031	00001	636	.00707	
8103.578	20033	10002	626	.00205	
8120.104	10032	00001	628	.00201	
8128.783	20032	10001	626	.00071	
8135.886	11132	01101	626	.0402	
8192.556	10032	00001	626	.424	
8220.363	10031	00001	628	.00201	
8243.163	20031	10001	626	.00108	
8254.800	12231	02201	626	.00164	
8276.767	11131	01101	626	.0461	
8293.957	10031	00001	626	.614	
9388.990	20033	00001	626	.00415	
9478.051	21132	01101	626	.00180	
9516.970	20032	00001	626	.0233	
9631.350	20031	00001	626	.0093	

Notes to Table IV-2.2

Bands deriving all their intensity from J-dependent perturbation are designated o pert, when one near band provides the intensity, π, when the listed intensity is multiplied by m(m+1), and Δ, when the listed intensity is multiplied by m^2 $(m+1)^2$.

Q designates bands with intensity below the criterion limit, whose Q - branches are significant.

of ζ^v included in Table 9. Note that when ζ_v is larger than 0.01, the total band strength, if defined as the sum of the Q, R- and P-branch lines, $\sum_m S_m$, may be much larger than S^o_v, its value when $\zeta_v = 0$. The entry in Table 10 is S^o_v, not $\sum_m S_m$.

As a higher-order effect of Coriolis interactions, transitions with $\ell' - \ell'' = \pm 2$ also become allowed, the effect increasing as m^2, so that a few such bands are intense enough to appear; here we list the value of S^o_v in the formula $S_m = S^o_v (|m| + m^2) \exp[(-1.439E'')/T]/Q_r$.

There are also a few special cases of near-or crossing-perturbations, where a normally very weak band "borrows" intensity from a stronger neighbor. A notable example is represented by the bands at 4808.186 cm^{-1}, where the 40002-01101 band with zero intensity, resonates with the 21113-01101 band at 4807.692 cm^{-1}. The positions and intensities of the individual lines are here calculated using an appropriate Coriolis constant and dividing the strength of 21113-01101 according to the degree of perturbational mixing.

4.2.3 CO_2 LINE HALF-WIDTHS

The half-widths for CO_2 were assigned by a linear function of the rotational quantum number. The work of Yamamoto, Tanaka and Aoki (1969) gave methods of estimating half-widths for the 15 μm and 4.3 μm regions, but the differences between their limited comparisons of calculated values and laboratory measurements did not seem to warrant any more complicated procedure in arriving at a half-width dependence upon J for CO_2.

4.3 Ozone

The band centers and intensities of all bands included in the compilation are given in Table 11.

The pure rotational transitions of ozone have been calculated using the molecular constants of Lichtenstein, Gallagher, and Clough (1971) obtained from microwave measurements. Transitions with upper state J less than 61 and intensities greater than 3.5×10^{-24} $cm^{-1}/mol\text{-}cm^2$ have been tabulated using a value of $\mu = 0.53D$ for the dipole moment. Lines with K_a less than 10 should be accurate to 0.001 cm^{-1}. Multiplets up to $K_a = 12$ ($\approx$100 cm^{-1}) have been observed and the calculated contours agree within the experimental accuracy (see Gebbie et al, 1966). At higher values of K_a, the calculations become increasingly less certain. However, even the highest value of K_a included in the listing (that is, $K_a = 20$) is substantially less than the value of K for which the calculation is divergent. The mean line width has been determined to be 0.11 (Lichtenstein et al, 1971).

Table 11. Ozone Transitions Included in Data Compilation

Band Center cm^{-1}	$\Sigma_i S_i$ $\frac{cm^{-1}}{mol/cm^2}$	Vibrational Transition		Isotope
		Upper State	Lower State	
0.	4.13×10^{-19}	000	000	666
700.930	6.70×10^{-19}	010	000	666
1007.693	9.49×10^{-21}	101	100	666
1007.996	2.49×10^{-20}	001	000	686
1021.096	4.23×10^{-19}	011	010	666
1027.096	1.62×10^{-19}	002	001	666
1028.096	5.16×10^{-20}	001	000	668
1042.096	1.29×10^{-17}	001	000	666
1103.157	3.47×10^{-19}	100	000	666
2110.790	1.33×10^{-18}	101	000	666
2785.241	2.32×10^{-20}	111	000	666
3041.200	1.10×10^{-19}	003	000	666

For the ν_2 fundamental of ozone, upper-state molecular constants have been obtained from microwave data by Tanaka and Morino (1970a). For a discussion of the determination of the band center see Tanaka and Morino (1970b). Transitions up to J = 60 with intensities greater than 3.5×10^{-23} $cm^{-1}/mol\text{-}cm^2$ have been tabulated. The dipole moment constant for the ν_2 fundamental has been taken as $(\partial\mu/\partial q_2)\, q_2 = 0.048D$ giving a band intensity of $6.76\ 10^{-19} cm^{-1}/mol\text{-}cm^2$ based on the measurements of McCaa and Shaw (1968).

The ν_3 and ν_1 regions of the ozone spectrum have been studied by Clough and Kneizys (1965, 1966), and Tanaka and Morino (1968). The positions of the ν_1 and ν_3 transitions for the main isotope are expected to be accurate to 0.01 cm^{-1} for J less than 40 and K_a less than eight with a degradation of accuracy for higher values of the quantum numbers. In conformity with the results of McCaa and Shaw (1968), the band intensity of ν_3 has been taken as 130×10^{-19} $cm^{-1}/mol\text{-}cm^2$.

Also, more lines have been included than were given in the report of Clough and Kneizys (1965). Goldman, et al (1970) have found that the absorption by large ozone amounts could not be satisfactorily explained without introducing the hot bands and the isotopic bands. Since the energy levels are known for the 101, the 100 and the 010 vibrational levels, transitions for the 101 ← 100 and 101 ← 001 bands may be calculated directly. The line positions for these bands with J less than 30 and K_a less than six are presumed accurate to ± 0.03 cm^{-1}. The line positions for the 011 ← 010 hot band have been obtained by applying a calculated shift of -21.0 cm^{-1} to the ν_3 transitions of the main isotope. For J less than 30 and K_a less than six an error of up to 1 cm^{-1} may be expected. For the 002 ← 001 hot band, a calculated shift of -15.0 cm^{-1} has been applied to the ν_3 transitions of the main isotope. In this case, the rotational levels of the upper- and lower-vibrational states are not accurately described, and these lines must be considered to be useful only for their general contribution to the low-resolution absorption in the region. These shifts have been calculated using harmonic frequencies and anharmonic corrections determined from an analysis of the available vibrational data.

For the 668 and 686 isotopes, shifts of -13.1 cm^{-1} and -34.1 cm^{-1} respectively have been determined from force constant calculations using the structural constants given by Tanaka and Morino (1968). These shifts have similarly been applied to the original ν_3 line calculations, neglecting the isotopic effect on the rotational constants. Consequently, only the general contribution to low-resolution spectra by these lines is valid. The intensities of the hot bands and the isotopic bands have been determined by applying the appropriate Boltzmann correction, isotopic abundance factor, dipole moment matrix element value, and degeneracy factor to the intensities of the ν_3 fundamental.

Although the addition of the isotopic bands and the hot bands gives improved agreement between calculated absorption and the observed absorption for large ozone amounts, it appears that an intensity anomaly still exists. In the P branch region ($\sim$ 1000 cm^{-1}) the calculated intensity is evidently too low, while in the R branch region the calculated intensity is too high. Until better intensity measurements are available, it will be difficult to obtain experimental F factors (see Section 3.2).

The ($\nu_1 + \nu_3$) combination band (101 ← 000) has been observed and analyzed using the rigid rotor approximation by Trajmar and McCaa (1964). The value of the band center was found to be 2110.79 cm^{-1}. The resolution and calibration accuracy of the observed spectra were not good, so that the line positions up to J = 20 and $K_a = 4$ are accurate to only 0.3 cm^{-1}. The error in line position is expected to be significantly greater for higher quantum numbers. The band intensity for the tabulated lines is $1.19 \times 10^{-18} \frac{\text{cm}^{-1}}{\text{mol/cm}^2}$.

The ($\nu_1 + \nu_2 + \nu_3$) combination band (111 ← 000) at 2785.241 has been studied by Snider and Shaw (1971). The rigid rotor analysis used gives line positions for J less than 25 and K_a less than 6 accurate to 0.1 cm^{-1}. The intensity for this band is $2.46 \times 10^{-20} \frac{\text{cm}^{-1}}{\text{mol/cm}^2}$ and was also obtained from McCaa and Shaw (1968).

Constants for the $3\nu_3$ band (003 ← 000) have been obtained from a second order calculation using the results of Tanaka and Morino (1968). The band intensity has been taken as 1.12×10^{-19} cm^{-1}/molecule-cm^{-2} from McCaa and Shaw (1968). The accuracy of the line positions should not be in error by more than ± 5 cm^{-1}.

4.4 Nitrous Oxide

Nitrous oxide is an asymmetric linear molecule (N-N-O) with three fundamental vibration-rotation bands, ν_1, ν_2, and ν_3, at 1284.907, 588.767, and 2223.756 cm^{-1}, respectively, for the main isotope. As for CO_2, $\nu_1 \cong 2\,\nu_2$ so that Fermi resonance occurs between these two levels, causing shifts of the band centers from the positions otherwise expected. Five different isotopes provide significant absorption. When no reference to a particular isotope is made, the most abundant one, 446, is implied. The abbreviated notations and natural abundances of each isotope used to calculate intensities of the isotopic bands are (446), 99.043 percent; (456), 0.358 percent; (546), 0.358 percent; (448), 0.199 percent; and (447), 0.040 percent. These values differ slightly from those given in Table 4, the difference arising from slight differences in the oxygen and nitrogen natural abundances taken from the 48th edition and the 42nd edition of the Handbook of Physics and Chemistry.* The 48th edition values were used in the construction of Table 4. These abundance differences are very small, but can be accounted for by modifying the line intensities accordingly.

4.4.1 LINE POSITIONS

Table 12 lists the constants used to calculate the line positions. Values of the vibrational energy, G, are relative to the 00^00 level for each isotope and are probably accurate to a few thousandths of a cm^{-1} for the 446 isotope. The uncertainty is much greater for some of the levels of the rarer isotopes. The majority of the constants for the 446 isotope and a few for the other isotopes are from Pliva (1964, 1968a, 1968b). Most of the other values have been derived by Benedict (private communications) from a variety of data.

Line positions for the P- and R-branches can be calculated by inserting the constants from Table 12 into Eq. (6). The selection rules are: $\Delta J = 0, \pm 1$; $\Delta \ell = 0, \pm 1$; and $J = 0 \nleftrightarrow J = 0$. The allowed values of J for a given vibrational level must be taken into account in order to determine missing lines. For example, in a $\Phi \leftarrow \Delta$ band ($\ell' = 3 \leftarrow \ell'' = 2$) the following lines are missing because of rotational energy levels that are not allowed: P1, P2, P3, Q0, Q1, Q2, R0 and R1.

A few lines of the 10^01, 06^00, 06^20, and $10^01 \leftarrow 10^00$ bands are shifted from the positions based on the constants in Table 12 because of Fermi interactions. These are discussed in more detail below and summarized in Table 15.

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*Published by the Chemical Rubber Co., Cleveland, Ohio

Table 12. Vibrational Energy Levels and Molecular Constants for N_2O

Energy Level	G (cm^{-1})	B (cm^{-1})	D Multiply by 10^{-7} (cm^{-1})	H Multiply by 10^{-12} (cm^{-1})
		Isotope 446		
$00^{0}0$	0	0.4190113	1.795	1.17
$01^{1c}0$	588.767	0.4191777	1.785	1.17
$01^{1d}0$	588.767	0.4199695	1.785	1.17
$02^{0}0$	1168.134	0.4199193	2.445	1.17
$02^{2c}0$	1177.750	0.4201253	1.165	1.17
$02^{2d}0$	1177.750	0.4201253	1.795	1.17
$10^{0}0$	1284.907	0.4172563	1.775	1.17
$03^{1c}0$	1749.058	0.4196063	2.195	1.17
$03^{1d}0$	1749.058	0.4210883	2.195	1.17
$03^{3d}0$	1766.958	0.420674	1.805	2.20
$03^{3c}0$	1766.958	0.420674	1.805	0.14
$11^{1c}0$	1880.268	0.4174673	1.765	1.17
$11^{1d}0$	1880.268	0.4183803	1.775	1.17
$04^{0}0$	2322.570	0.4206113	4.095	16.17
$04^{2c}0$	(2331.15)	0.4210113	1.350	1.17
$04^{2d}0$	(2331.15)	0.4210113	2.50	1.17
$12^{0}0$	2461.998	0.4181483	2.465	3.77
$12^{2c}0$	2474.785	0.4187143	1.210	1.17
$12^{2d}0$	2474.785	0.4187143	1.700	1.17
$20^{0}0$	2563.341	0.4224193	1.645	1.17
$00^{0}1$	2223.756	0.4155613	1.795	1.17
$05^{1c}0$	2897.876		2.085	1.17
$05^{1d}0$	2897.876		2.355	1.17
$13^{1c}0$	3046.213	0.4177633	2.145	1.17
$13^{1d}0$	3046.213	0.4193783	2.165	1.17
$13^{3c}0$	3067.749	0.419109	1.805	0.47
$13^{3d}0$	3067.749	0.419109	1.805	1.87

Table 12. Vibrational Energy Levels and Molecular Constants for N_2O (Contd)

Energy Level	G (cm^{-1})	B (cm^{-1})	D Multiply by 10^{-7} (cm^{-1})	H Multiply by 10^{-12} (cm^{-1})
		Isotope 446 (Contd)		
$21^{1c}0$	3165.857	0.4158333	1.595	1.17
$21^{1d}0$	3165.857	0.4169163	1.595	1.17
$01^{1c}1$	2798.290	0.4157723	1.795	1.17
$01^{1d}1$	2798.290	0.4165473	1.795	1.17
$14^{0}0$	3620.941	0.4187873	3.885	14.17
$14^{2c}0$	3631.601	0.4190143	0.375	1.17
$14^{2d}0$	3631.601	0.4190143	2.045	1.17
$22^{0}0$	3748.252	0.4163273	2.395	2.77
$22^{2c}0$	3766.060	0.4172013	1.200	1.17
$22^{2d}0$	3766.060	0.4172013	1.560	1.17
$30^{0}0$	3836.373	0.4141473	1.385	1.17
$02^{0}1$	3363.974	0.4165443	2.445	1.17
$02^{2c}1$	3373.137	0.4167523	1.195	1.17
$02^{2d}1$	3373.137	0.4167523	1.795	1.17
$10^{0}1$	3480.821	0.4137843	1.745	1.17
$23^{1c}0$	4335.798	0.4159193	2.045	1.17
$23^{1d}0$	4335.798	0.4176813	2.115	1.17
$31^{1c}0$	4446.379	0.4143703	1.625	1.17
$31^{1d}0$	4446.379	0.4156713	1.365	1.17
$03^{1c}1$	3931.258	0.4162253	1.915	1.17
$03^{1d}1$	3931.258	0.4176843	1.925	1.17
$03^{3c}1$	3948.344	0.417327	1.815	0.14
$03^{3d}1$	3948.344	0.417327	1.815	2.20
$11^{1c}1$	4061.979	0.4140513	1.775	1.17
$11^{1d}1$	4061.979	0.4149343	1.735	1.17
$40^{0}0$	5105.65	0.4131913	1.795	1.17
$32^{0}0$	5026.34	0.4143113	1.795	1.17
$20^{0}1$	4730.828	0.4121163	1.625	1.17
$12^{0}1$	4630.164	0.4147633	2.475	4.17
$12^{2c}1$	4642.463	0.4151583	1.315	1.17
$12^{2d}1$	4642.463	0.4151583	1.315	1.17
002	4417.379	0.4120963	1.765	1.17

Table 12. Vibrational Energy Levels and Molecular Constants for N_2O (Contd)

Energy Level	G (cm^{-1})	B (cm^{-1})	D Multiply by 10^{-7} (cm^{-1})	H Multiply by 10^{-12} (cm^{-1})
		Isotope 446 (Contd)		
$21^{1c}1$	5319.175	0.4124313	1.675	1.17
$21^{1d}1$	5319.175	0.4134703	1.555	1.17
$01^{1c}2$	4977.695	0.4123583	1.785	1.17
$01^{1d}2$	4977.695	0.4131183	1.785	1.17
		Isotope 456		
$00^{0}0$	0	0.4189821	1.75	
$01^{1c}0$	575.5	0.419095	1.75	
$01^{1d}0$	575.5	0.419891	1.75	
$10^{0}0$	1280.5	0.41719	1.72	
$11^{1c}0$	1861.9	0.41734	1.71	
$11^{1d}0$	1861.9	0.41820	1.70	
$20^{0}0$	2554.3	0.41545	1.67	
$00^{0}1$	2177.659	0.41568	1.75	
$01^{1c}1$	2739.63	0.415855	1.75	
$01^{1d}1$	2739.63	0.416605	1.75	
$10^{0}1$	3430.95	0.41387	1.72	
		Isotope 546		
$00^{0}0$	0	0.4048564	1.64	
$01^{1c}0$	585.320	0.4050304	1.65	
$01^{1d}0$	585.320	0.4057724	1.65	
$10^{0}0$	1269.894	0.403269	1.60	
$11^{1c}0$	1863.080	0.4034614	1.59	
$11^{1d}0$	1863.080	0.4043814	1.57	
$20^{0}0$	2534.21	0.401870	1.45	
$00^{0}1$	2201.604	0.401495	1.65	
$01^{1c}1$	2745.709	0.4017054	1.65	
$01^{1d}1$	2745.709	0.4024104	1.65	
$10^{0}1$	3443.659	0.399876	1.60	

Table 12. Vibrational Energy Levels and Molecular Constants for N_2O (Contd)

Energy Level	G (cm^{-1})	B (cm^{-1})	D Multiply by 10^{-7} (cm^{-1})	H Multiply by 10^{-12} (cm^{-1})
Isotope 448				
00^00	0	0.395577	1.65	
$01^{1c}0$	584.1	0.395749	1.65	
$01^{1d}0$	584.1	0.396461	1.65	
10^00	1247.9	0.394057	1.55	
$11^{1c}0$	1839.8	0.39430	1.56	
$11^{1d}0$	1839.8	0.39513	1.50	
20^00	2491.3	0.39279	1.31	
00^01	2218.97	0.392317	1.65	
$01^{1c}1$	2788.80	0.392549		
$01^{1d}1$	2788.80	0.393209		
10^01	3439.1	0.39078	1.55	
Isotope 447				
00^00	0	0.406691	1.72	
$01^{1c}0$	586.3	0.406860	1.72	
$01^{1d}0$	586.3	0.407610	1.72	
10^00	1265.5	0.405961	1.67	
00^01	2221.3	0.40334		
$01^{1c}1$	2793.55	0.40357		
$01^{1d}1$	2793.55	0.40430		

4.4.2 LINE INTENSITIES

Each band system contains a main band and associated hot bands that arise from transitions from excited energy levels with the same changes Δv_1, Δv_2, and Δv_3 in the vibrational quantum numbers as in the main band. The change $\Delta \ell$ may be either 0 or $\pm$ 1 within the same band system. For example, the 0^01 band is the main band in a system that also contains the hot bands $01^11 \leftarrow 01^10$, $02^01 \leftarrow 02^00$, $02^21 \leftarrow 02^20$, $10^01 \leftarrow 10^00$, and many others from higher excited energy levels. The relative intensities of the hot bands decrease with increasing value of the lower energy level because of the decrease in its population. Thus, only a few of the hot bands are usually significant. Corresponding bands of the rare isotopic molecules are also part of the system. The main band of the common isotope accounts for 78 percent to 89 percent of the entire system for 296°K samples, depending on the band system.

Table 13 summarizes the normal band systems containing lines with intensities greater than 4×10^{-23} molecules $^{-1}$ cm^2 cm^{-1}. Each band system is identified by the main band whose center position is given. The intensities are based on recent measurements of the quantity $\int (-1/u) \ln T \, d\nu$ by Burch et al, (1971a, 1971b, 1971c, 1972). The integration was performed over the entire band system, and u is the N_2O thickness in molecules cm^{-2}. The intensity, S_Q, of only the Q-branch of the band at 1974.571 cm^{-1} is listed because the P and R branches contain no lines with intensities above the cut-off. The Q-branch may be significant although each of its lines is very weak because they occur very close together. Bands containing the 06^00 and 06^20 levels are not listed because the band systems are very weak. However, as a result of Fermi interaction between a few of the rotational levels, the intensities of the corresponding lines are anomalously high and their positions are shifted. These lines are discussed in more detail below.

Table 14 lists the intensities of each of the bands with lines above the cutoff intensity, nominally 4×10^{-23} molecules $^{-1}$ cm^2 cm^{-1}. Each line entry in the table corresponds to a given band, and blank lines occur before and after each band system. Note that 16 bands are listed for the 00^01 band system, whereas only 1 or 2 bands are listed for some of the weaker systems.

Each rotational level within a vibrational level for which quantum number $\ell \neq 0$ is split into two sublevels normally indicated by "c" and "d" (see section 3.1.1). A band involving two Δ levels, or two π levels, or one of each level consists of two sub-bands, one from the c portion of the lower level and one from the d portion. The $c \leftarrow c$ portion of the first sub-band contains only P- and R-branches, whereas the $d \leftarrow c$ portion contains the Q-branch. Similarly, the $d \leftarrow d$ and the $c \leftarrow d$ portions of the second sub-band contain the P + R branches and the Q-branch, respectively. The intensities, S_v, given in Table 14 are the total for both sub-bands.

Table 13. Summary of N_2O Band Systems

Center of Main Band (cm^{-1})	Upper Level	Lower Level	Intensity of System Multiply by 10^{-20} $Molecules^{-1}\ cm^{2}\ cm^{-1}$
588.767	$01^{1}0$	$00^{0}0$	118 ± 9
696.140	$10^{0}0$	$01^{1}0$	0.354 ± 0.020
938.849	$00^{0}1$	$10^{0}0$	0.254 ± 0.010
1168.134	$02^{0}0$	$00^{0}0$	38.5 ± 1.5
1284.907	$10^{0}0$	$00^{0}0$	996 ± 40
1634.989	$00^{0}1$	$01^{1}0$	0.278 ± 0.02
1749.058	$03^{1}0$	$00^{0}0$	0.241 ± 0.02
1880.268	$11^{1}0$	$00^{0}0$	1.66 ± 0.08
1974.571	$20^{0}0$	$01^{1}0$	S_Q = 0.024 ± 0.002
2223.756	$00^{0}1$	$00^{0}0$	5710 ± 250
2322.624	$04^{0}0$	$00^{0}0$	2.7 ± 0.3
2461.998	$12^{0}0$	$00^{0}0$	33.4 ± 1.5
2563.341	$20^{0}0$	$00^{0}0$	135 ± 7
2798.290	$01^{1}1$	$00^{0}0$	9.62 ± 0.96
3363.974	$02^{0}1$	$00^{0}0$	10.6 ± 0.5
3480.821	$10^{0}1$	$00^{0}0$	197 ± 10
3620.941	$14^{0}0$	$00^{0}0$	0.56 + 0.02, - 0.05
3748.252	$22^{0}0$	$00^{0}0$	4.12 ± 0.2
3836.373	$30^{0}0$	$00^{0}0$	8.15 ± 0.4
4061.979	$11^{1}1$	$00^{0}0$	0.111 ± 0.006
4335.798	$23^{1}0$	$00^{0}0$	0.1 + 0.1, - 0.07
4417.379	$00^{0}2$	$00^{0}0$	6.9 ± 0.7
4630.164	$12^{0}1$	$00^{0}0$	0.68 ± 0.07
4730.828	$20^{0}1$	$00^{0}0$	4.4 ± 0.4
4977.695	$01^{1}2$	$00^{0}0$	0.070 ± 0.008
5026.34	$32^{0}0$	$00^{0}0$	0.29 ± 0.04
5105.65	$40^{0}0$	$00^{0}0$	0.29 ± 0.03

Table 14. N_2O Band Intensities

Band Center ν_c (cm^{-1})	Upper Level	Lower Level	Isotope	S_v at 296K (Multiply by 10^{-20} Molecules^{-1} cm^{2}cm^{-1})
588.767	$01^{1}0$	$00^{0}0$	446	98.4
579.367	$02^{0}0$	$01^{1}0$	446	4.90
588.983	$02^{2}0$	$01^{1}0$	446	11.26
580.924	$03^{1}0$	$02^{0}0$	446	0.599
571.308	$03^{1}0$	$02^{2}0$	446	0.256
589.208	$03^{3}0$	$02^{2}0$	446	0.958
595.361	$11^{1}0$	$10^{0}0$	446	0.216
585.320	$01^{1}0$	$00^{0}0$	546	0.356
575.5	$01^{1}0$	$00^{0}0$	456	0.356
586.3	$01^{1}0$	$00^{0}0$	447	0.039
584.1	$01^{1}0$	$00^{0}0$	448	0.197
696.140	$10^{0}0$	$01^{1}0$	446	0.294
938.849	$00^{0}1$	$10^{0}0$	446	0.223
1168.134	$02^{0}0$	$00^{0}0$	446	31.7
1160.291	$03^{1}0$	$01^{1}0$	446	5.72
1154.436	$04^{0}0$	$02^{0}0$	446	0.201
1153.40	$04^{2}0$	$02^{2}0$	446	0.228
1177.750	$02^{2}0$	$00^{0}0$	446	See Note A
1284.907	$10^{0}0$	$00^{0}0$	446	872.
1291.501	$11^{1}0$	$01^{1}0$	446	100.6
1293.864	$12^{0}0$	$02^{0}0$	446	3.16
1297.035	$12^{2}0$	$02^{2}0$	446	5.92
1278.434	$20^{0}0$	$10^{0}0$	446	3.73
1297.155	$13^{1}0$	$03^{1}0$	446	0.390
1300.791	$13^{3}0$	$03^{3}0$	446	0.364
1285.589	$21^{1}0$	$11^{1}0$	446	0.412
1280.5	$10^{0}0$	$00^{0}0$	456	3.15
1286.4	$11^{1}0$	$01^{1}0$	456	0.354
1269.894	$10^{0}0$	$00^{0}0$	546	3.15
1277.760	$11^{1}0$	$01^{1}0$	546	0.362
1247.9	$10^{0}0$	$00^{0}0$	448	1.75
1255.7	$11^{1}0$	$01^{1}0$	448	0.200
1265.5	$10^{0}0$	$00^{0}0$	447	0.350
1634.989	$00^{0}1$	$01^{1}0$	446	0.231
1749.058	$03^{1}0$	$00^{0}0$	446	0.200
1880.268	$11^{1}0$	$00^{0}0$	446	1.41
1886.018	$12^{2}0$	$01^{1}0$	446	0.156
1873.231	$12^{0}1$	$01^{1}0$	446	0.053
1974.571	$20^{0}0$	$01^{1}0$	446	$S_Q = 0.024$
2181.66	$06^{0}0$	$10^{0}0$	446	See Note B

Table 14. N_2O Band Intensities (Contd)

Band Center ν_c (cm^{-1})	Upper Level	Lower Level	Isotope	S_v at 296K (Multiply by 10^{-20} Molecules^{-1} $cm^2 cm^{-1}$)
2223.756	00^01	00^00	446	5023.
2209.523	01^11	01^10	446	568.
2195.840	02^01	02^00	446	16.8
2195.387	02^21	02^20	446	31.8
2195.914	10^01	10^00	446	10.1
2182.200	03^11	03^10	446	1.958
2181.386	03^31	03^30	446	1.88
2181.711	11^11	11^10	446	1.10
2193.623	00^02	00^01	446	0.201
2177.659	00^01	00^00	456	18.1
2164.13	01^11	01^10	456	2.04
2201.604	00^01	00^00	546	18.1
2187.389	01^11	01^10	546	2.10
2218.97	00^01	00^00	448	10.1
2204.70	01^11	01^10	448	1.15
2221.3	00^01	00^00	447	2.01
2207.25	01^11	01^10	447	0.234
2322.624	04^00	00^00	446	2.11
2309.109	05^10	01^10	446	0.54
2461.998	12^00	00^00	446	27.6
2457.446	13^10	01^10	446	4.68
2452.807	14^00	02^00	446	0.239
2453.851	14^20	02^20	446	0.321
2463.345	22^00	10^00	446	0.192
2563.341	20^00	00^00	446	120.
2577.090	21^10	01^10	446	12.2
2580.118	22^00	02^00	446	0.348
2588.310	22^20	02^20	446	0.648
2551.466	30^00	10^00	446	0.696
2534.21	20^00	00^00	546	0.454
2554.3	20^00	00^00	456	0.384
2491.3	20^00	00^00	448	0.192
2474.785	12^20	00^00	446	See Note A
2798.290	01^11	00^00	446	8.06
2775.207	02^01	01^10	446	0.401
2784.370	02^21	01^10	446	0.912
2763.124	03^11	02^00	446	0.025
2753.508	03^11	02^20	446	0.020
2770.594	03^31	02^20	446	0.078
3363.074	02^01	00^00	446	8.82
3342.491	03^11	01^10	446	1.57

Table 14. N_2O Band Intensities (Contd)

Band Center ν_c (cm^{-1})	Upper Level	Lower Level	Isotope	S_v at 296K (Multiply by 10^{-20} $Molecules^{-1}\ cm^2 cm^{-1}$)
3480.821	10^01	00^00	446	173.
3473.212	11^11	01^10	446	19.24
3462.030	12^0_21	02^0_20	446	0.563
3464.713	12^21	02^20	446	1.064
3445.921	20^01	10^00	446	0.652
3443.659	10^01	00^00	546	0.627
3430.95	10^01	00^00	456	0.627
3439.1	10^01	00^00	448	0.348
3466.54	06^0_20	00^00	446	See Note B
3474.65	06^20	00^00	446	See Note A and B
3748.252	22^0_10	00^0_10	446	3.52
3747.031	23^10	01^10	446	0.512
3620.941	14^00	00^00	446	0.492
3836.373	30^00	00^00	446	7.28
3857.612	31^10	01^10	446	0.698
4061.979	11^11	00^00	446	0.092
4335.798	23^10	00^00	446	0.083
4417.379	00^02	00^00	446	6.07
4388.928	01^12	01^10	446	0.686
4630.164	12^01	00^00	446	0.597
4730.828	20^01	00^00	446	3.90
4730.408	21^11	01^10	446	0.410
4977.695	01^12	00^00	446	0.058
5026.34	32^00	00^00	446	0.255
5105.65	40^00	00^00	446	0.255

The intensities of the majority of the bands have been calculated from the experimental values for the entire band systems listed in Table 13. Calculating the intensity of an individual band from that of the entire band system involves the population of each energy level, the degeneracy of each level, and the relative transition probabilities.

In some of the band systems, the experimental results indicate that the transition probabilities are the same for all bands within a given system. However, as in the 12^00 band system, for example, the transition probabilities are greater for the $13^10 \leftarrow 01^10$ and $14^00 \leftarrow 02^00$ bands than for the 12^00 band. These differences in transition probabilities were found experimentally by comparing the relative intensities of several isolated lines within the system.

Equations relating the intensities of individual lines to that of the entire band are given in Section 3. These are applicable to the N_2O bands listed in Table 14 with the exception of two forbidden $\Delta \leftarrow \Sigma$ bands, 02^20 and 12^20, and those listed in Table 15. The factor ζ (see Section 3 Eq. (13)) that accounts for the Coriolis vibration-rotation interaction can be assumed to be zero for all bands in Table 14, except for the 03^10 and 11^10 bands; ζ equals approximately -0.01 and -0.007, respectively, for these bands.

Young (1972) has tabulated the relative intensities of the lines within a given band for which the Coriolis interaction is negligible. A large fraction of the intensity of a band system is in the main band; therefore, uncertainties in the relative transition probabilities within a band system do not seriously increase the uncertainty of the main-band intensity calculated on the basis of that of the entire band system. Thus, the percent of uncertainty in the intensity of the main band is approximately the same as that for the entire band system, whereas the uncertainty for the hot bands may be greater.

4.4.3 FORBIDDEN BANDS AND PERTURBED LINES

As a result of Coriolis interactions, transitions with $\ell' - \ell'' = \pm 2$ become allowed. Two N_2O bands of interest that arise from such "forbidden" transitions are the $02^20 \leftarrow 00^00$ and $12^20 \leftarrow 00^00$ bands centered at 1177.750 and 2474.785 cm^{-1}, respectively. The relationship between the intensities of the individual lines within a band is different for these bands than for normal bands. As in the case of CO_2, the intensities are given by Eq. (15) where $S_v^o = 1.36 \times 10^{-5}$ molecules^{-1} cm^2 cm^{-1} for the $02^{2c}0$ band and $S_v^o = 9.5 \times 10^{-6}$ molecules^{-1} cm^2 cm^{-1} for the $12^{2c}0$ band.

A few rotational levels of the 06^00 vibrational state (centered at J = 46) and the 06^20 state (centered at J = 28) are perturbed by the corresponding levels of the 10^01 state to such an extent that the normally very weak lines "borrow" enough

Table 15. Parameters of Perturbed Lines of N_2O

Line	Band	ν_o (cm^{-1})	S_J $\times 10^{-20}$ $molecules^{-1}$ cm^2 cm^{-1}
R45	10^01	1)3508.030	0.207
R45	06^00	2)3508.186	0.046
P47	10^01	1)3430.230	0.136
P47	06^00	2)3430.400	0.031
R27	10^01	1)3500.040	2.11
R27	06^20	2)3499.970	0.0233
P29	10^01	1)3452.330	1.71
P29	06^20	2)3452.260	0.0188
R45	$10^01 \leftarrow 10^00$	3)2226.713	0.0118
P47	$10^01 \leftarrow 10^00$	3)2149.246	0.0042

1) The perturbed line positions of the 10^01 band are from observed values by Tidwell et al, (1960).

2) The calculated positions of perturbed lines of the 06^00 and 06^20 bands were determined from known perturbed positions of the 10^01 lines and Toth's (1971a) values of the line separations.

3) The calculated positions of the perturbed $10^01 \leftarrow 10^00$ lines were determined from Toth's (1971a) results and the positions of the unperturbed lines calculated on the basis of the constants in Table 12.

4) The perturbed line intensities of the 06^00 and 06^20 bands are based on the intensities of the unperturbed lines of the 10^01 band and Toth's (1971a) results. The unperturbed line intensities of the 10^01 and $10^01 \leftarrow 10^00$ bands are based on the band intensities given in Table 13 and Young's (1972) relative line intensities.

intensity from the 10^01 lines to appear, at the same time shifting the positions of the lines related to these rotational levels (Toth, 1971a). The resulting positions and intensities of the affected lines have been calculated separately and are given in Table 15. The R27 and R29 lines of the $10^01 \leftarrow 10^00$ band are not listed in the table because the changes in their intensities and positions are negligible.

4.4.4 LINE HALF-WIDTHS

Several workers have measured the half-widths of N_2O lines broadened by N_2, which is a good approximation to broadening by air. Toth (1971b) has recently measured the widths of lines in the R branches of the 10^01 and 02^01 bands directly from observed spectra with a small correction for the effect of the spectrometer slitwidth. Margolis (1972) has used the same method to measure the lines in both the P- and R-branches of the 00^02 band. The results of these two workers are in good agreement, indicating that there is little, if any, dependence on vibrational mode. Lowder's (1972) recent measurements on the $00^{0}1$ band show approximately the same dependence on J as do the results of Toth and Margolis, although Lowder's values averaged approximately 10 percent less. Oppenheim and Goldman (1971) have measured half-widths indirectly by applying band models to low-resolution spectra of a wide variety of N_2O samples. Their results are in fair agreement with those of Margolis and Toth. Fraley et al, (1962) reported an average value of 0.05 cm^{-1} atm^{-1} for lines in the $00^{0}1$ band; this value is considerably lower than those reported by the workers mentioned above.

We have adopted half-widths of N_2-broadened lines reported by Toth (1971b) to be used for atmospheric N_2O lines near 296°K. A few values are listed in the tabulation below; values for other J's can be found by interpolation and for other temperatures by assuming the half-widths are inversely proportional to the square root of temperature.

J	^{o} cm^{-1} atm^{-1}
1	0.0915
4	0.0948
10	0.0892
20	0.0812
30	0.0767
40	0.0748
50	0.0698
60	0.0604

4.5 Carbon Monoxide

For the CO bands, we have depended heavily on the work of Young (1968). Table 16 provides the rotational constants which were used to compute the line positions of the main isotope. The positions of the less abundant isotopes were computed from the appropriate constants for the 26 isotope by applying the ratio of reduced masses. The accuracy of the line positions in the main isotope is expected to be about ± 0.001 cm^{-1}. The accuracy of the line positions of the other isotopes will be somewhat less, about ± 0.01 cm^{-1}.

The intensities for the fundamental and first two overtone bands were taken from Young and are reproduced in Table 17. The intensities for the isotopic bands were taken to be the same as for the 26 isotope reduced by the relative abundances given in Table 4 and the square of the frequency. The intensity of the fundamental appears to be known very accurately, perhaps within ± 2 percent; the first overtone is less accurately known to ± 10 percent; and the second overtone is known to ± 4 percent (see Young and Eachus, 1966); Burch and Gryvnak (1967). Half-width values have been added to the compilation following the work of Hunt et al, (1968).

Table 16. Rotational Constants Used in the Calculation of CO Line Positions

Symbol	Value
ω_e	2169.836
$\omega_e X_e$	13.295
$\omega_e Y_e$	0.0115
B_e	1.931285
α_e	0.017535
γ_e	1.01×10^{-5}
D_c	6.12×10^{-6}
β_e	1.0×10^{-9}

Table 17. Intensities of CO Bands

	1-0	2-0	3-0
Intensity, S(cm^{-1}/molecule-cm^{-2})	9.70×10^{-18}	6.99×10^{-20}	4.83×10^{-22}

4.6 Methane

This molecule is a spherical top, in the rigid rotor approximation. It has tetrahedral (T_d) symmetry in the rest configuration of its nuclei. Rotation-vibration interactions are complicated even for its simplest infrared-active bands. Starting from the molecular Hamiltonian and the electric dipole-moment operator, transition energies, selection rules, and intensities may be calculated. However, the techniques and the results are complex, and it is not convenient to summarize them here. Therefore, the user is referred to the original papers on this subject John (1968), Schaffer et al, (1939), Hecht (1960), Moret-Bailly (1961), Herranz (1961), Fox (1962), Dang-Nhu (1969), and Susskind (1972).

For the purpose of the present data compilation, we have established the following conventions in notation. The isotopic species $^{12}CH_4$, $^{13}CH_4$, and $^{12}CH_3D$ are denoted by the digits 211, 311, and 212, respectively, in columns 75 through 77. The quantum numbers for the initial and final states of a transition are specified in columns 36 through 69 as follows:

$v'_1v'_2\ell'_2v'_3\ell'_3v'_4\ell'_4\ell'$	$v''_1v''_2\ell''_2v''_3\ell''_3v''_4\ell''_4\ell''$	J'R'	C'	N'	J"R"	C"	N"
1X 8I1	1X 8I1	1X 2I2	1A1 1I1	1I1	1X 2I2	1A1 1I1	1I1

except for type E symmetry which has for C the format 1X 1A1 instead of 1A1 1I1. The initial and final state vibrational and rotational quantum numbers have their usual meanings. To avoid ambiguity, we establish some further conventions for the present data compilation. The selection rule C' ← C" on T_d symmetry is always taken to be $A_1 \leftarrow A_2$, $A_2 \leftarrow A_1$, $E \leftarrow E$, $F_1 \leftarrow F_2$, or $F_2 \leftarrow F_1$. The numbering scheme for the N's begins with 1, 2, 3 . . . Whenever possible, N increases with increasing ground-state energy; the stronger lines correspond to the selection rule, N' - N'' = 0.

This section describes methane spectral data in the 3 to 8.5 μm region. The following bands, as summarized in Table 18, have been included: ν_2, ν_3, ν_4, $\nu_2 + \nu_4$, $2\nu_4$.

Table 18. Methane Bands Included in Data Compilation

Isotope	Band	Center (cm^{-1})	Upper State	Lower State	Intensity ($cm^{-1}/mole\text{-}cm^{-2}$)
311	ν_4	1297.88[a]	00000111	00000000	6.59×10^{-20}[h]
211	ν_4	1305.9138[b]	00000111	00000000	5.87×10^{-18}[i]
211	ν_2	1533.289[c]	01100001	00000000	8.91×10^{-20}[i]
311	ν_3	3009.53[d]	00011001	00000000	1.36×10^{-19}[h]
211	ν_3	3018.9205[e]	00011001	00000000	1.21×10^{-17}[i]
211	$2\nu_4$	2600[f]	00000222	00000000	1×10^{-19}[j]
211	$\nu_2 + \nu_4$	2818, 2838[g]	01100112	00000000	8×10^{-19}[h]

a. Kyle et al, (1970)
b. Michelot and Fox (1973)
c. Dang-Nhu (1968)
d. McDowell (1966)
e. Bobin and Fox (1973)
f. Fox (1973)
g. Benedict (1973)
h. 1/89 times value for corresponding band of 211 isotope
i. Armstrong and Walsh (1960)
j. 1/100 times value for ν_3 of 211 isotope
k. 1/15 times value for ν_3 of 211 isotope

It is planned to add other weak but significant bands in this spectral region at a later time.

Many line positions, together with their absolute intensities and widths, have been included in the present data compilation, even though the corresponding quantum number assignments are uncertain or unknown at this time. It must be stressed that much of the needed theoretical and experimental research on spectra of methane is still incomplete. Consequently, a large portion of the data compilation should be considered tentative and subject to revision at a later time.

4.6.1 LINE POSITIONS

The band ν_3 at 3.3 μm is the strongest infrared-active vibration-rotation fundamental of CH_4. High-resolution measurements of line positions for $^{12}CH_4$ in the range 2884 to 3141 cm^{-1} have been used. See Henry et al, (1970), and Barnes et al, (1972). Quantum number assignments for the allowed lines from 2840 to 3167 cm^{-1} were made by Bobin and Fox (1973) on the basis of fourth-order perturbation theory. Some forbidden lines were assigned by Barnes et al, (1972) using third order theory. Spectroscopic parameters determined for the ground-state and for ν_3 of CH_4 are listed in Tables 19 and 20, respectively. The corresponding band of the isotopic species $^{13}CH_4$ has been measured from 2873 to 3123 cm^{-1}. The assignments of McDowell (1966) with some modifications were used. The corresponding spectroscopic parameters are listed in Table 23.

Table 19. Spectroscopic Parameters for Ground State of $^{12}CH_4$

Parameter	Value (cm^{-1})
B	5.24059 ± 0.00006[a]
D_s	$(1.086 \pm 0.003) \times 10^{-4}$[a]
D_t	$(4.403 \pm 0.099) \times 10^{-6}$[b]

a. Barnes et al, (1972)
b. Ozier et al, (1970). The error bar is derived from the values given by Barnes et al, (1972) and Husson and Dang Nhu (1971).

The band at 7.7 μm is the next strongest fundamental of $^{12}CH_4$. High-resolution measurements in the 1225 to 1393 cm^{-1} range made by Botineau (1972) were used to obtain spectral line positions. Quantum-number assignments for the allowed lines, to J=12 for the R and Q branches, and J=13 for the P branch, were made by Michelot and Fox, (1973) on the basis of a fourth order calculation. For J=13 to 15 in the Q branch only, and for some J=13 R-branch lines, quantum-number assignments were taken from the work of Husson and Poussigue (1971). No forbidden lines of this band have been included in the data compilation yet. The determined spectroscopic parameters are given in Table 21. For ν_4 of $^{13}CH_4$, the measurements of Kyle et al, (1970), extend from 1226 to 1359 cm^{-1}, and possibly further. The assignments of Kyle et al, (1970) with some modifications were used; spectroscopic parameters appear in Table 24.

Table 20. Spectroscopic Parameters* for ν_3 of $^{12}CH_4$

Parameter	Value (cm^{-1})	Parameter	Value (cm^{-1})
m	3018.9205	g	4.265×10^{-3}
n	9.87157	h	8.365×10^{-5}
p	-4.0622×10^{-2}	k	-1.925×10^{-5}
q	-2.959×10^{-4}	ℓ	2.509×10^{-7}
s	4.329×10^{-5}	j	5.84×10^{-8}
t	1.942×10^{-7}	u	2.605×10^{-5}
x	-9.11×10^{-8}	z	-5.39×10^{-8}
v	-4.7921×10^{-2}	z'	1.49×10^{-6}
w	3.622×10^{-5}	z''	7.08×10^{-8}

*Bobin and Fox (1973)

Table 21. Spectroscopic Parameters* for ν_4 of $^{12}CH_4$

Parameter	Value (cm^{-1})	Parameter	Value (cm^{-1})
m	1305.9138	g	1.8643×10^{-2}
n	5.5752	h	6.590×10^{-4}
p	-6.4192×10^{-2}	k	2.88×10^{-6}
q	1.91×10^{-3}	ℓ	1.67×10^{-7}
s	1.479×10^{-6}	j	-3.78×10^{-9}
t	-1.11×10^{-6}	u	2.077×10^{-5}
x	-1.79×10^{-8}	z	-1.18×10^{-8}
v	-5.2263×10^{-2}	z'	-1.901×10^{-6}
w	2.319×10^{-5}	z''	8.28×10^{-8}

*Michelot and Fox (1973)

The ν_2 fundamental at 6.5 μm is relatively weakly infrared-active, by virtue its Coriolis interaction with ν_4. Quantum-number assignments are based on the results of Dang Nhu (1969) who developed a fourth-order theory and applied it to unpublished spectra of moderately high resolution. Spectroscopic parameters are listed in Table 22.

High-resolution spectra of $\nu_2 + \nu_4$ and $2\nu_4$ are available in the region of approximately 2450 to 3200 cm^{-1} (Plyler et al, 1960; and Hall, 1973). Quantum-number assignments for $2\nu_4$ have been made on the basis of a third-order theoretical analysis. A partial analysis of $\nu_2 + \nu_4$ has been done in analogy with the quantum-number assignments in the work of (Bregier, 1970; and Hilico, 1970), on $\nu_2 + \nu_3$. Spectroscopic parameters for $\nu_2 + \nu_4$ and $2\nu_4$ are given in Tables 25 and 26 respectively.

Table 22. Spectroscopic Parameters* for ν_2 of $^{12}CH_4$

Parameter	Value (cm^{-1})
v_2	1533.289
B_2	5.319
B_o	5.230
d_2	5.7×10^{-5}
d_o	2.1×10^{-5}
z_2	2.9×10^{-2}
f_2	-5.2×10^{-3}
e_2	-2.8×10^{-5}
e_o	-5.0×10^{-6}

*Dang Nhu (1968)

Table 23. Spectroscopic Parameters* for ν_3 of $^{13}CH_4$

Parameter	Value (cm^{-1})
$\nu_o - 2(B\zeta_3)eff$	3009.05 ± 0.03
$B_o + B_{eff}^{P,Q} - 2(B\zeta_3)_{eff}$	9.963 ± 0.004
$B_{eff}^{P,R} - B_o$	-0.0386 ± 0.0008
$2(D_o + D_1)$	$(4.2 \pm 0.4) \times 10^{-4}$
$D_o - D_1$	$(2.1 \pm 0.5) \times 10^{-5}$
δ_3	0.046 ± 0.005
$D^{J\tau}$	$(4.7 \pm 2.8) \times 10^{-5}$
$d^{J\tau}$	$(5.4 \pm 1.7) \times 10^{-5}$

*McDowell (1966)

Table 24. Spectroscopic Parameters* for ν_4 of $^{13}CH_4$

Parameter	Value (cm^{-1})
ν_4	1297.88 ± 0.02
B	5.179 ± 0.005
B'	5.194 ± 0.005
D	$(1.16 \pm 0.02) \times 10^{-4}$
ξ	0.477 ± 0.005
F_{4s}	$(2.26 \pm 0.02) \times 10^{-3}$
t_{044}	-4.5×10^{-6}
t_{134}	$(4.84 \pm 0.02) \times 10^{-4}$
t_{224}	$(-1.46 \pm 0.01) \times 10^{-2}$

*Kyle et al, (1970)

Table 25. Spectroscopic Parameters* for $\nu_2 + \nu_4$ of $^{12}CH_4$

Parameter	Value (cm^{-1})
$\nu_o(Q)$	2818, 2838

*Hiliev (1970) - Further analysis, including that of the interaction between F_1 and F_2 substates, is necessary in order to obtain more complete values of spectroscopic parameters.

Table 26. Spectroscopic Parameters* for $2\nu_4$ of $^{12}CH_4$

Parameter	Value (cm^{-1})
ϵ	2600.29
B	5.175
$B\zeta$	2.520
D	1.0×10^{-4}
G_{44}	3.1
g	1.837×10^{-2}
h	6.579×10^{-4}

*Fox (1962)

4.6.2 LINE INTENSITIES

Although it is recognized that it would be desirable to include in the data compilation all methane lines whose absolute intensity exceeds the cutoff specified in Table 3, it has not been possible to achieve this goal because of present experimental and theoretical limitations.

Absolute intensities for the allowed lines in ν_3 of $^{12}CH_4$ were calculated, starting from the measured values for R(0); R(1), and R(2). The relative intensities of forbidden lines (Barnes et al, 1972) were used for calculating their absolute intensities. The absolute line intensities for ν_3 of $^{13}CH_4$ were calculated on the basis of those for ν_3 of $^{12}CH_4$, together with the terrestrial $^{12}C/^{13}C$ ratio (see Table 4). Calculated and/or measured absolute band intensities are listed in Table 18.

Absolute line intensities for ν_4 have been calculated on the basis of the measured values for R(0), R(1), and R(2). For $^{13}CH_4$, absolute intensities were calculated as for ν_3. Absolute band intensities are given in Table 18.

Absolute line intensities for ν_2, have been calculated on the basis of theoretical relative-line intensities and the experimental absolute band intensity in Table 18.

Absolute-line intensities for $\nu_2+\nu_4$ were determined from the solar spectra of Hall (1972), with an assumed CH_4 air mass of approximately 4×10^{19} molecules/cm^2 and an assumed temperature of 273°K and a pressure of 0.65 atm.

Absolute line intensities for $2\nu_4$ were calculated from the relative intensity formula of Fox (1962) together with the absolute band intensity in Table 18. The latter intensity was taken to be approximately 1/100 of that for ν_3 of $^{12}CH_4$.

4.6.3 LINE WIDTHS

The J- and T-dependence of methane line widths is taken from the results of Varanasi et al, (1971, 1972) and Tejwani and Varanasi (1971). The only measured values of air-broadened CH_4 half-widths are for multiples of ν_3 and $2\nu_3$ at T= 295°K. For $J \approx 1$ to 5, $\gamma^o \approx 0.061$ cm^{-1} atm^{-1}; for $J \approx 15$ to 17, $\gamma^o \approx 0.048$ cm^{-1} atm^{-1}. These results agree with values calculated from γ^o for CH_4-O_2, assuming N_2 and O_2 with their partial pressures in air. Measurements and calculations of γ^o for CH_4-H_2 in ν_4 suggest, but do not prove directly, that γ^o may be independent of vibration-rotation band. For the purpose of the present data compilation, we adopt the value $\gamma^o = 0.055$ cm^{-1} atm^{-1} for all CH_4 lines. There are no results available for the T-dependence of γ^o for CH_4-air or even CH_4-N_2 or CH_4-O_2 broadening. From the calculations and measurements for CH_4-H_2 broadening with T, we assume the usual $T^{-1/2}$ dependence. In conclusion, for the present data compilation, we use

$$\gamma^o = 0.055\left(\frac{296}{T}\right)^{1/2}\left(\frac{p}{1 \text{ atm}}\right). \tag{16}$$

4.7 Oxygen

The infrared atmospheric bands of oxygen have been interpreted by Van Vleck as magnetic dipole transitions between intersystem electronic combinations, a singlet-triplet transition $a^1\Delta_g \leftarrow X\,^3\Sigma_g^-$. The Δ v=0 (0,0) band at 7882.39 cm^{-1} (1.27 μm) has an Einstein A coefficient of 1.9×10^{-4} sec^{-1} Jones and Harrison (1958) . The (0,0) band, and the weaker (1,0) band at 9365.89 cm^{-1} have been observed in terrestial atmospheric absorption by Herzberg and Herzberg (1947). The (0,1) band at 6325.99 cm^{-1} has been observed in the twilight airglow emission by Jones and Harrison (1958). In addition to these bands there is an electric quadrupole ($b^1\Sigma^+_g$-$a^1\Delta_g$) transition at 1.908 μm that has been detected in the emission spectrum of a discharge through O_2 and helium (Noxon, 1961). Finally, submillimeter-wave rotational transitions (McKnight and Gordy, 1968) and spin reorientation spectra (Zimmerer and Mizushima, 1961) at 60 GHz have been observed in the ground electronic state. The (a-X) system and the microwave spectra are discussed below. The atmospheric "A" band at 7619Å, representing the magnetic dipole transition $b^1\Sigma_g^+ \leftarrow X^3\,\Sigma_g^-$, is also included (Wark and Mercer, 1965; Burch and Gryunak, 1967).

With the molecular rotational momentum designated by $\utilde{K}$ and the electronic spin vector by $\utilde{S}$, the total angular momentum $\utilde{J}$ is given by

$$\utilde{J}=\utilde{K}+\utilde{S}.$$

Thus, for the singlet-delta state J=K, and the energy levels, apart from the vibration, are given by

$$F = B_vK(K+1) - D_vK^2(K+1)^2, \tag{17}$$

where B_v is the rotational constant and D_v is the first order centrifugal distortion constant for the particular vibrational state. The constants for this state, obtained from measurements of the infrared bands, are listed in Table 27.

The expressions for the rotational energies of the rho-type triplet are obtained from a solution of the Hamiltonian (West and Mizushima, 1966):

$$H = B\,\utilde{K}^2 + \frac{2}{3}\,\lambda(3S_z^2 - \utilde{S}^2) + \mu\utilde{K}\cdot\utilde{S}, \tag{18}$$

where λ is the spin-spin interaction coupling constant and μ is the spin-rotation interaction coupling constant.

Table 27. Constants of the $^1\Delta_g$ State of 0_2 (Herzberg and Herzberg, 1947)

Constant	Value (in cm^{-1})
B_o	1.41783
B_1	1.4007
D_o	4.86×10^{-6}
ω_e	1509.3
$\omega_e x_e$	12.9
$\Delta G_{1/2}$	1483.50
ν_e	7918.134

Centrifugal stretching effects are approximately corrected for by assuming a K(K+1) dependence for B, λ and μ, namely:

$$B = B_v - D_v K(K+1) + H_v K^2(K+1)^2,$$

$$\lambda = \lambda_o - \lambda_1 K(K+1), \text{ and}$$

$$\mu = \mu_o - \mu_1 K(K+1). \qquad (19)$$

For each value of the quantum number at end-over-end rotation, K, the triplet energies are given by $F_1(K)$, $F_2(K)$, and $F_3(K)$ where J = K+1, J=K and J=K-1, respectively. Both $F_1(K)$ and $F_3(K)$ average about 2 cm^{-1} lower than the $F_2(K)$ component. Values for the constants of the triplet-sigma state, obtained from both infrared and microwave measurements, are given in Table 28.

The band centers are given by

$$G(v',v'') = \nu_e + \omega_e'(v'+1/2) - \omega_e' x_e'(v'+1/2)^2 + \ldots - \omega_e''(v''+1/2) +$$

$$\omega_e'' x_e''(v''+1/2)^2 - \omega_e'' y_e''(v''+1/2)^3 + \omega_e'' z_e''(v''+1/2)^4 + \ldots, \qquad (20)$$

where the prime and double primes refer to the singlet and triplet states respectively.

The selection rules for magnetic dipole radiation are

$$\Delta J = 0, \pm 1$$

and

$$+ \leftrightarrow +,\ - \leftrightarrow -,\ g \leftrightarrow g,\ u \leftrightarrow u.$$

Table 28. Constants for the $^3\Sigma_g^-$ State of O_2

Constant	Reference	Value (cm^{-1})
B_o	a	1.4376809
B_1	b	1.421979
D_o	b	4.913×10^{-6}
D_1	b	4.825×10^{-6}
H_o	b	3.0×10^{-10}
λ_o	c	1.9847530
λ_1	c	-1.950×10^{-6}
μ_o	c	-8.42930×10^{-3}
μ_1	c	8.01×10^{-9}
ω_e	b	1580.3613
$\omega_e x_e$	b	12.0730
$\omega_e y_e$	b	5.46×10^{-2}
$\omega_e z_e$	b	-1.43×10^{-3}
$\Delta G_{1/2}$	b	1556.3856

a. McKnight and Gordy (1968)
b. Babcock and Herzberg (1948)
c. West and Mizushima (1966)

The possible branches and the nomenclature used here for the $^1\Delta_g \leftarrow {}^3\Sigma_g^-$ transition are shown in Table 27. Since the oxygen-16 nuclei obey Bose-Einstein statistics, only the positive rotational levels occur. In the ground state this causes an alternation of lines such that only odd values of the rotational quantum number K are present. For the heteronuclear isotopes of oxygen, however, all rotational levels occur; the $O^{17}O^{17}$ molecule has alternate rotational levels with nuclear statistical weights of 5 and 7 (Gordy et al, 1953). In $O^{16}O^{16}$ (and $O^{18}O^{18}$) there are four branches with $\Delta K=\pm1$, three with $\Delta K=0$, and two with $\Delta K=\pm2$, the latter branches being designated by superscripts S and O. On the magnetic tape the six quantum numbers of the transition, v', J', K', v'', J'', K'', are given in the field of columns 38 through 62. In addition, the nine branches are listed in columns 64 and 65 with the superscript, representing the ΔK of the transition, preceding the ΔJ designation. A diagram indicating the transitions involved in the $^1\Delta_g \leftarrow {}^3\Sigma_g^-$ band is given in Figure 1.

The above description generally applies to the microwave transitions of pure rotation and transitions between levels of the triplet state. In the latter the labelling is given as K+ and K-, designating the transitions $F_2(K) - F_1(K)$ and $F_2(K) - F_3(K)$ respectively. Intensities have been calculated (see Townes and Schawlow, 1955). A good summary of the various bands of oxygen molecule can be found in the recent review article by Krupenie, 1972.

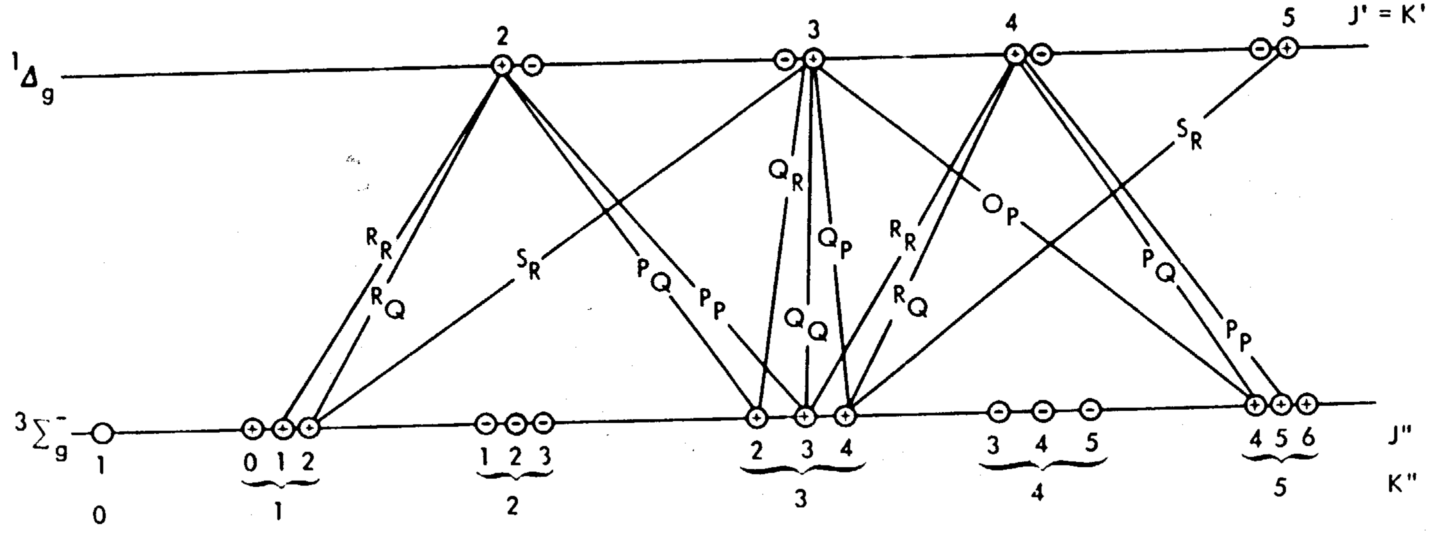

Figure 1. Transitions in the $^1\Delta_g \leftarrow {}^3\Sigma_g^-$ Band of Oxygen

5. CONTINUOUS ABSORPTION BY ATMOSPHERIC GASES

Although not part of the data tape of primary concern in this report, a few words should be said about the relatively continuous regions of absorption of particular interest in the atmospheric "windows" near 2500 cm^{-1} (4 μm), from approximately 1250 cm^{-1} to 700 cm^{-1} (8 μm - 14 μm), and near 450 cm^{-1} (22 μm). In other spectral regions the contribution by nearby absorption lines is much greater than that by the continuum absorption, so that for practical purposes the continuum effect can be neglected, although it may be greater than in the windows.

This continuous absorption is caused by one or more of the following three processes: (1) extreme wings of strong collision-broadened absorption lines centered more than 10-20 cm^{-1} away; (2) pressure induced absorption resulting from transitions that are forbidden for unperturbed molecules; and (3) the possible existence of the water dimer ($H_20:H_20$) in the case of the 8 to 14 μm region.

The absorption coefficient due to continuum absorption can be expressed as

$$k = C_s P + C_b P_b \qquad (22)$$

where C_s is the self-broadened coefficient and C_b is the foreign gas broadening coefficient, P is the total pressure and P_b is the foreign gas pressure.

Figure 2 gives the spectral dependence of C_s for water vapor absorption in the 8 to 14 μm region for three temperatures (Burch, 1970). The C_b value has been most reliably measured by McCoy et al, 1969, and is found for nitrogen to be $C_b = 0.005C_s$ at room temperature.

Figure 3 gives the spectral dependence of C_s for the water vapor absorption in the region near 4 μm for four different temperatures (Burch et al, 1971a). Note that the $T=296^{o}K$ curve is an extrapolation based on the measurements at higher temperature. These same workers found the ratio C_b/C_s for nitorgen broadening to be 0.12 ± 0.03.

Figure 4 gives the spectral dependence of the absorption coefficient due to the pressure-induced nitrogen absorption centered near 2330 cm^{-1} (Burch et al, 1971a). Measurements have also been made by Shapiro and Gush, 1966, and Farmer and Houghton, 1966. Since the foreign gas broadening in this case results from a gas (oxygen) having a constant mixing ratio in the atmosphere, Eq. (22) reduces to

$$K = \text{Const.} \times P \qquad (23)$$

Since the nitrogen abundance in the atmosphere is also directly proportional to P, the absorption depends on P^2 and Figure 4 has as ordinate the absorption coefficient expressed in the units $atm^{-2}\ Km^{-1}$.

Since line wings as given by the Lorentz shape, Eq. (1), have been found to be in error in the extreme wings, an appropriate rule to follow for the truncation of

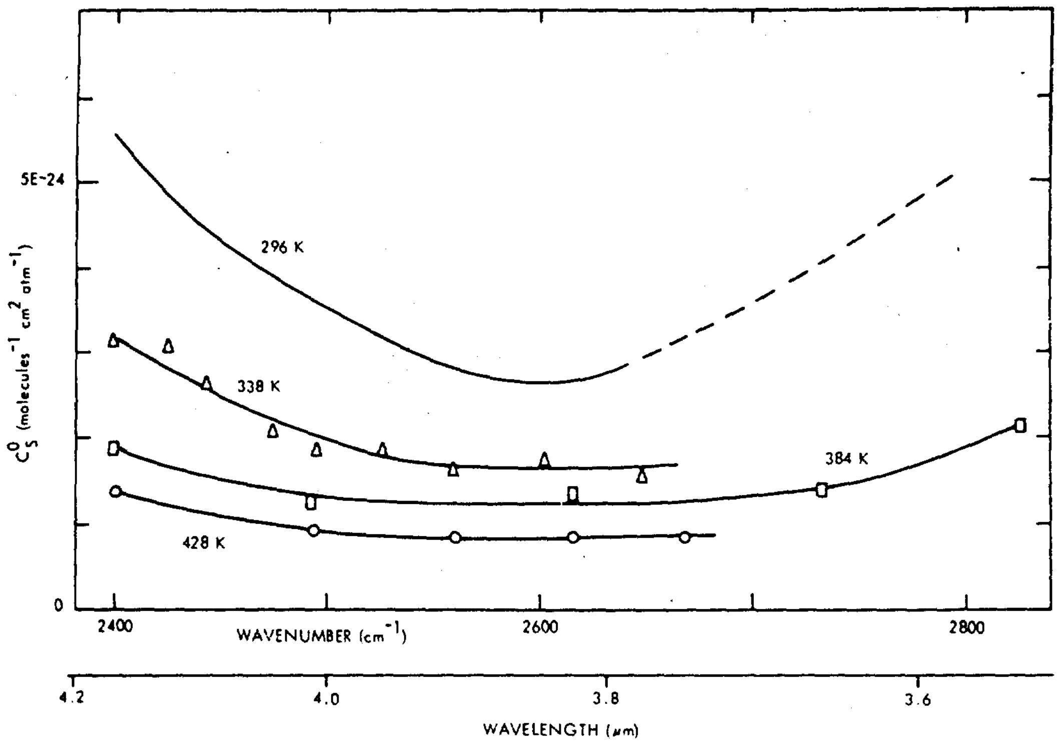

Figure 2. Normalized Continuum Absorption Coefficient for H_2O at Three Temperatures

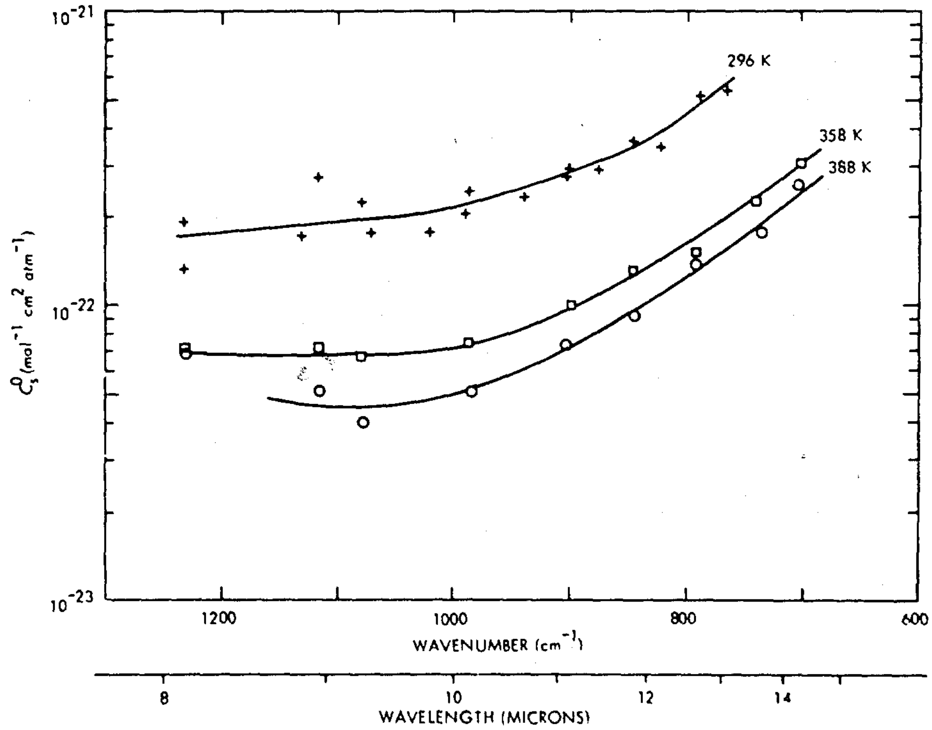

Figure 3. Normalized Continuum Absorption Coefficient Between 2400 and 2820 cm^{-1} for Pure H_2O at Four Temperatures

line wings and the introduction of continuum absorption coefficients in accordance with Figures 2 through 4 is difficult to state. It is recommended that the user familiarize himself with this problem (see, for example, Burch et al, 1969) and in any case the use of the Lorentz shape beyond 20 or 30 wavenumbers of line centers is inappropriate (see also discussion on line shape on p. 3).

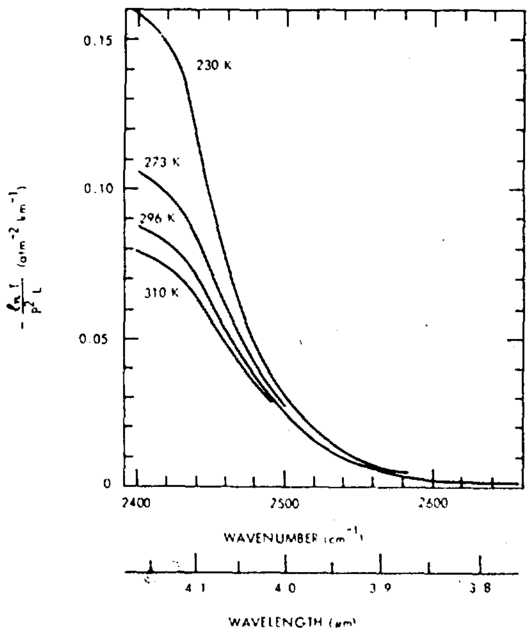

Figure 4. Spectral Plot of Absorption Coefficient for Atmospheric N_2 at Four Temperatures

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Appendix A

Computer Program Listing for Reading Tape

```
      PROGRAM RD TP( INPUT, OUTPUT, TAPE2)
      DIMENSION R(400),TT(15)
       A=0
      IEOF=0
   24 BUFFER IN(2,0) (R(1),R(390))
      IF(UNIT(2)) 25,30,35
   35 PRINT 35,TT(1)
   36 FORMAT(* PARITY ERROR  AFTER *,F12.3)
      GO TO 24
   30 IEOF=IEOF+1
      PRINT 31,IEOF
   31 FORMAT(* EOF NO*,I5)
       IF(IEOF.GT.7) GO TO 1001
       GO TO 24
   25 DECODE(10,39,R(1))IRED
   41 FORMAT(F10.3,E10.3,F5.3,F10.3,5A6,A5,I3,I4,I3)
      I=1
   39 FORMAT(I10)
      L=2
      DO 40 K=1,IRED
      DECODE(80,41,R(L))(TT(I),I=1,13)
      PRINT 41,(TT(I),I=1,13)
      L=L+8
      IF(TT(1).LT.A) PRINT 153,A,TT(1)
       A=TT(1)
 153  FORMAT(* OUT OF ORDER *,2F12.3)
   40 CONTINUE
      GO TO 24
 1001 CALL EXIT
        STOP
       END
```

Appendix B

Computer Program for Homogeneous Path Transmittance Calculation

The computer program (Program LBL) provided in this Appendix is intended for use as a check to ensure that a user of the AFCRL Data Tape will be using the data correctly. The spectral region chosen for a sample spectrum (Figure 5) contains spectral lines from four different atmospheric gases. The program was constructed for use with constant pressure and temperature paths only, so the user will be left to his own devices for real atmospheric applications. After computing transmittance at closely spaced monochromatic frequencies, a convolution is performed over a triangular slit function whose half-width can be chosen. Comment cards have been used freely, so no further discussion of this program will be given here.

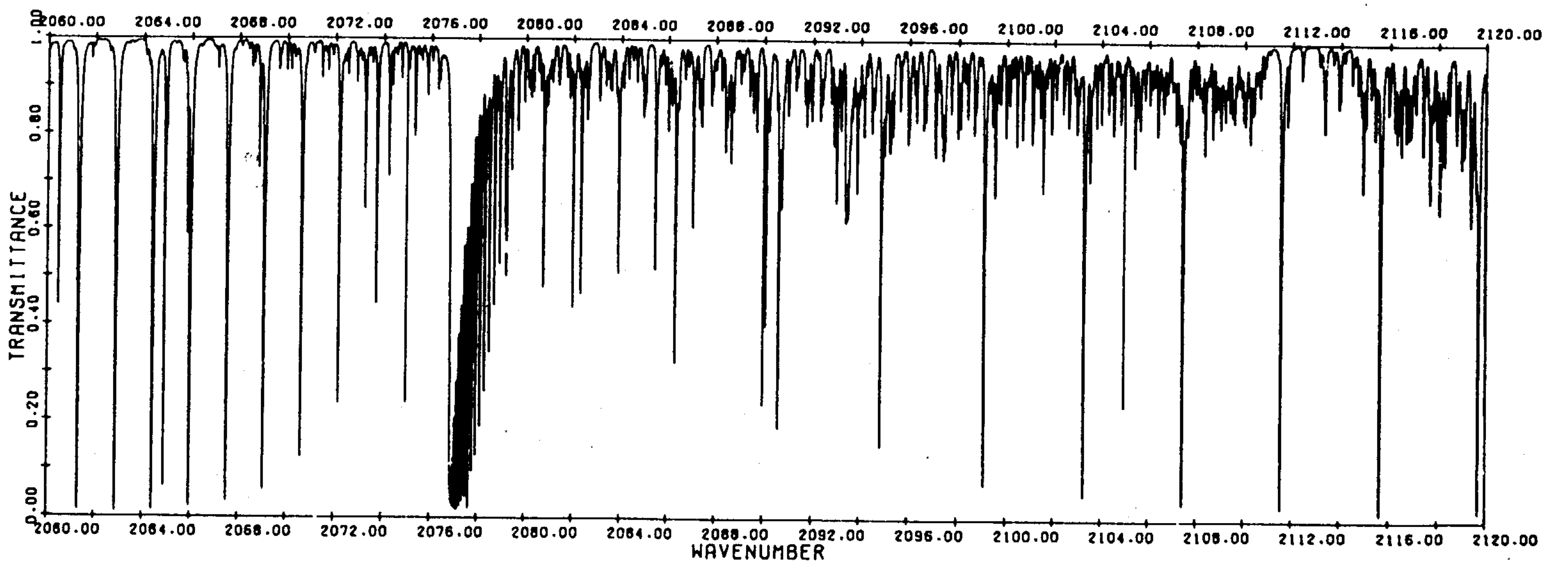

Figure B1

Synthetic Spectrum Generated using the Data Compilation. Conditions are as follows: pressure = 188 mb, T = 219K, W H_2O = 2.00×10^{20}, $W_{CO_2} = 2.05 \times 10^{21}$, $W_{O_3} = 3.23 \times 10^{18}$, $W_{CO} = 4.67 \times 10^{17}$. Lines belonging to other molecular species contained on tape are not present in this spectral region. Spectral resolution is 0.01 cm^{-1}.

```
      PROGRAM LBL(INPUT,OUTPUT,TAPE2)
      DIMENSION W(7), R(325), GNU(3000), S(3000), ALPHA(3000), EDP(3000)
      DIMENSION MOL(3000), CAY1(7), OPD(3000), FNU(1000), TRANS(1000)
      DIMENSION SUM1(7), CS2(7)
C
C     PROGRAM BY R. MCCLATCHEY.
C
C     NO PUNCHED DECKS WILL BE DISTRIBUTED.
C
C     THIS PROGRAM GENERATES A TRANSMITTANCE SPECTRUM WITH OUTPUT RESULTS
C     PRINTED EVERY DELV WAVENUMBERS BETWEEN THE INITIAL FREQUENCY,
C     V1, AND THE FINAL FREQUENCY,V2.  CALCULATIONS ARE PERFORMED FOR
C     A UNIFORM, CONSTANT PRESSURE, CONSTANT TEMPERATURE PATH CONTAINING
C     ANY OR ALL OF THE MOLECULAR SPECIES DESCRIBED IN THIS REPORT
C     IN ARBITRARY AMOUNTS.  MOLECULAR ABUNDANCES MUST BE SPECIFIED
C     IN THE UNITS (MOLECULES/CM2).  MONOCHROMATIC CALCULATIONS ARE
C     MADE AT FREQUENCY INTERVALS,DV, AND A TRIANGULAR SLIT FUNCTION
C     OF HALF-WIDTH,A, IS CONVOLVED WITH THE MONOCHROMATIC RESULTS.
C
C
C
      IEOF=0
      DEPTH=0.001
      PI=3.14159
      SUM=0.0
      IV=1
C
C     READ INPUT PARAMETERS (P=PRESSURE), (T=TEMPERATURE),
C     W(1)=H2O, W(2)=CO2,W(3)=O3,W(4)=N2O,W(5)=CO,W(6)=CH4,W(7)=O2.
C     V1 AND V2 ARE FREQUENCY LIMITS FOR WHICH OUTPUT RESULTS ARE REQUIRED.
C     DV IS MONOCHROMATIC FREQUENCY INCREMENT.
C     BOUND IS THE FREQUENCY FROM ANY LINE CENTER BEYOND WHICH THE LINE
C     WILL BE NEGLECTED.
C     A IS THE HALF-WIDTH OF A TRIANGULAR SLIT FUNCTION.
C     DELV IS FREQUENCY INCREMENT OF CONVOLVED OUTPUT TRANSMITTANCE
C     RESULTS.
C
      READ 77, P,T
      PRINT 79, P,T
      READ 81, (W(M),M=1,7)
      PRINT 83
      PRINT 81, (W(M),M=1,7)
      READ 85, V1,V2,DV,BOUND,A,DELV
      PRINT 87, V1,V2,DV,BOUND,A,DELV
C     IF(A*2/DV+1.GT.3000) CALCULATION CANNOT BE DONE
C     IF THERE ARE MORE THAN 3000 LINES READ FROM TAPE IN A FREQUENCY RANGE
C     OF 2(A+BOUND) CALCULATION CANNOT BE DONE
      VBOT=V1-A-BOUND
      VTOP=V2+A+BOUND
      MFILE=0
      IF (VBOT.GE.500.0) MFILE=1
      IF (VBOT.GE.1000.0) MFILE=2
      IF (VBOT.GE.2000.0) MFILE=3
      IF (VBOT.GE.5000.0) MFILE=4
```

NOT REPRODUCIBLE

```
C
C     MFILE DETERMINES THE NUMBER OF ENDS OF FILE TO BE READ OVER
C     BEFORE COMING TO THE PERTINENT DATA ON THE TAPE.
C     WE ARE NOW READY TO READ TAPE.
C
      I=1
      ILL=1
1     BUFFER IN (2,0) (R(1),R(325))
      IF (UNIT(2)) 7,5,3
3     PRINT 89, GNU(I)
      GO TO 1
5     IEOF=IEOF+1
      PRINT 91, IEOF
      IF (IEOF.GE.7) GO TO 75
      GO TO 1
7     IF (MFILE.GT.IEOF) GO TO 1
      DECODE (10,93,R(1) )IREC
      NT=(8*IREC)-6
      DECODE (10,95,R(NT) )TMAX
      IF (TMAX.LT.VBOT) GO TO 1
      L=2
      DO 9 K=1,IREC
      DECODE (80,95,R(L) )GNU(I),S(I),ALPHA(I),EDP(I),IDAT,ISOT,MOL(I)
      L=L+8
      IF (GNU(I).LT.VBOT) GO TO 9
      M=MOL(I)
      PATH=S(I)*W(M)/(PI*0.06*P/1013.0)
      IF (PATH.LT.DEPTH) GO TO 9
      IF (GNU(I).GT.VTOP) GO TO 11
      I=I+1
9     CONTINUE
      IF (I.GT.2960) GO TO 11
      GO TO 1
11    I1=I
      PRINT 97, VBOT,VTOP,GNU(I1),I1
      I5=1
      V2P=GNU(I1)-BOUND-A
C
C     TAPE HAS BEEN READ FOR ALL NECESSARY LINES OR FOR THE MAXIMUM NO.
C     OF LINES POSSIBLE SUBJECT TO RECYCLING.
C     HALFWIDTHS WILL BE SUPPLIED BELOW WHEN THEY DO NOT APPEAR
C     ON TAPE.
C
      DO 15 I=ILL,I1
      M=MOL(I)
      IF (M.EQ.1) GO TO 15
      IF (ALPHA(I).GT.0.0) GO TO 13
      IF (M.EQ.2) ALPHA(I)=0.07
      IF (M.EQ.3) ALPHA(I)=0.11
      IF (M.EQ.4) ALPHA(I)=0.08
      IF (M.EQ.5) ALPHA(I)=0.06
      IF (M.EQ.6) ALPHA(I)=0.055
      IF (M.EQ.7) ALPHA(I)=0.048
13    IF (ALPHA(I).LT.0.01.OR.ALPHA(I).GT.1.0) ALPHA(I)=0.06
```

```
15    CONTINUE
      I5=1
      P0=1013.00
      T0=296.00
      CS1=(T0-T)/(T0*T*0.6946)
C
C     ROTATIONAL PARTITION FUNCTION IS DEFINED BELOW
C
      DO 21 M=1,7
      IF (M.EQ.1) GO TO 17
      IF (M.EQ.2) GO TO 19
      IF (M.EQ.3) GO TO 17
      IF (M.EQ.4) GO TO 19
      IF (M.EQ.5) GO TO 19
      IF (M.EQ.6) GO TO 17
      IF (M.EQ.7) GO TO 19
17    CS2(M)=((T0/T)**1.5)
      GO TO 21
19    CS2(M)=T0/T
21    CONTINUE
      CA=((T0/T)**0.5)*(P/P0)
C
C     TEMPERATURE DEPENDENCE OF ALL LINE INTENSITIES COMPUTED HERE.
C
      DO 23 I=ILL,I1
      M=MOL(I)
      S(I)=S(I)*CS2(M)*EXP(-EDP(I)*CS1)
23    ALPHA(I)=ALPHA(I)*CA
      V=V1-A
25    DO 27 M=1,7
      CAY1(M)=0.0
27    SUM1(M)=0.0
C
C     DETERMINE INDICES (I5 AND I6) INDICATING WHICH SPECTRAL LINES
C     ARE TO BE USED IN THE CALCULATION AT FREQUENCY V.
C
      DO 33 I=I5,I1
      IF (V-BOUND-GNU(I)) 29,29,33
29    I5=I
      GO TO 35
33    CONTINUE
      I5=I1
      GO TO 49
35    DO 39 J=I5,I1
      IF (V+BOUND-GNU(J)) 37,37,39
37    I6=J-1
      GO TO 43
39    CONTINUE
      I6=I1
C
C     COMPUTE THE OPTICAL DEPTH AND TRANSMITTANCE AT FREQUENCY V.
C
43    DO 45 I=I5,I6
      M=MOL(I)
```

```
      Z=ABS(V-GNU(I))
      SUM1(M)=S(I)*ALPHA(I)/(Z**2+ALPHA(I)**2)
      CAY1(M)=CAY1(M)+SUM1(M)
45    CONTINUE
      CAY=0.0
      DO 47 M=1,7
47    CAY=CAY+CAY1(M)*W(M)
      OPD(IV)=CAY*0.3183
      GO TO 51
49    OPD(IV)=0.0
51    OPD(IV)=EXP(-OPD(IV))
      IF ((V+DV).GT.V2P) GO TO 53
      IF (V.GE.V2+A) GO TO 53
      IF (IV.GE.3000) GO TO 53
      IV=IV+1
      V=V+DV
      GO TO 25
C
C     AT THIS POINT, CYCLE BACK TO STATEMENT 25 AND COMPUTE THE
C     MONOCHROMATIC TRANSMITTANCE AT V+DV,ETC.
C     IF STATEMENT 53 IS REACHED ,ALL POSSIBLE MONOCHROMATIC TRANSMITTANCE
C     VALUES HAVE BEEN COMPUTED, AND THE SLIT FUNCTION CONVOLUTION WILL
C     NOW BE PERFORMED IN LOOP 57
C
53    FREQ=V1
      PRINT 101, IV,V,V2P
      FINAL=V1+3000.*DV-A-DELV
      V=V1-A
      JFNU=1
      L=DELV/DV+0.01
      IA=1
55    SUM=0.0
      DO 57 I=IA,IV
      SUM=SUM+(A-ABS(V-FREQ))*OPD(I)
      V=V+DV
      IF (V-(FREQ+A)) 57,59,59
57    CONTINUE
59    TRANS(JFNU)=SUM*DV/(A*A)
      FNU(JFNU)=FREQ
      IF (FREQ.GT.V2) GO TO 61
      IF (FREQ.GT.V2P) GO TO 61
      IF (FREQ.GE.FINAL) GO TO 61
      FREQ=FREQ+DELV
      IF (JFNU.GE.1000) GO TO 61
      JFNU=JFNU+1
      IA=IA+L
      V=FREQ-A
      SUM=0.0
      GO TO 55
C
C     CONVOLVED TRANSMITTANCE RESULTS ARE NOW PRINTED OUT.
C
61    PRINT 103, JFNU
      PRINT 104
```

```
      PRINT 105, (FNU(J),TRANS(J),J=1,JFNU)
      IF (FREQ.GE.V2) GO TO 75
      IF (FREQ.GT.V2P) GO TO 67
      IF (JFNU.GE.1000) GO TO 65
      IF (FREQ.GE.FINAL) GO TO 63
      GO TO 75
63    V1=FINAL+DELV
      I5=1
      IV=1
      JFNU=1
      V=V1-A
      GO TO 25
65    IA=IA+L
C
C     IF STATEMENT 65 IS REACHED, ADDITIONAL MONOCHROMATIC CALCULATIONS
C     ARE REQUIRED TO SATISFY THE TOTAL FREQUENCY RANGE OVER WHICH
C     CONVOLVED RESULTS ARE REQUIRED.
C
      JFNU=1
      V=FREQ-A
      GO TO 55
67    IV=1
C
C     IF STATEMENT 67 IS REACHED, THE DATA FROM THE DATA TAPE WILL BE
C     REORGANIZED AND THE TAPE WILL BE READ AGAIN.
C
      JFNU=1
      V1=FREQ
      VBOT=V1-A-BOUND
      DO 69 IN=1,I1
      IF (GNU(IN).GT.VBOT) GO TO 71
69    CONTINUE
      IN=I1
71    IJ=IN
      L=1
      DO 73 I=IJ,I1
      GNU(L)=GNU(I)
      S(L)=S(I)
      ALPHA(L)=ALPHA(I)
      EOP(L)=EOP(I)
      MOL(L)=MOL(I)
73    L=L+1
      I=L
      ILL=L
      GO TO 1
75    CALL EXIT
      STOP
C
77    FORMAT (E12.5,F7.2)
79    FORMAT (* PRESSURE =*,E12.5,*TEMPERATURE =*,F7.2)
81    FORMAT (7E10.3)
83    FORMAT (3X,*WATER*,5X,*CO2*,6X,*OZONE*,7X,*N2O*,7X,*CO*,8X,*CH4*,7
     1X,*O2*,4X)
85    FORMAT (6F10.3)
```

NOT REPRODUCIBLE

```
87    FORMAT (* V1 =*,F10.3,*V2 =*,F10.3,*DV=*,F10.3,*BOUND =*,F10.3,*A
     1=*,F10.3,*DELV =*,F10.3)
89    FORMAT (* PARITY ERROR ENCOUNTERED AT*,F12.3)
91    FORMAT (* END OF FILE ENCOUNTERED*,I5)
93    FORMAT (I10)
95    FORMAT (F10.3,E10.3,F5.3,F10.3,35X,I3,I4,I3)
97    FORMAT (* VBOT =*,F12.3,* VTOP =*,F12.3,*GNU =*,F12.3,* I1 *,I8)
101   FORMAT (I5,2F10.4)
103   FORMAT (* JFNU =*,I5)
104   FORMAT (5(* FREQUENCY   TRANS.    *))
105   FORMAT (5(F10.3,E12.5))
      END
```