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ABSORPTION COEFFICIENTS OF SULFUR DIOXIDE MICROWAVE ROTATIONAL LINES

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Abstract

New calculations of the frequencies and absorption coefficients of the rotational transitions of $^{32}S^{16}O_2$ are given for all energy levels up to J = 50 and frequencies less than 200 GHz. A spectrometer incorporating a semi-confocal Fabry-Perot resonant cavity and operating in the vicinity of 70 GHz is described. The calculated absorption coefficients are compared to measured values obtained with this spectrometer and to existing measurements over the frequency range 26-40 GHz. The results obtained are in general agreement to within 5 to 10 per cent. A detailed knowledge of the absorption coefficient behavior as a function of frequency is of particular interest in the development of high-sensitivity SO_2 monitors, and investigations of the kinetics of fast chemical reactions.

Introduction

The technique of microwave spectroscopy offers an attractive method (1, 2) for the study of pollutant gases of environmental interest. The polar molecule SO_2 is of particular interest, both because it is an important pollutant and because it exhibits relatively strong absorptions at microwave frequencies. For the purposes of pollutant monitoring or investigations of the kinetics of chemical reactions, it is desirable to select the transitions within a given frequency range having the strongest intensities. While the microwave spectrum of SO_2 has been extensively studied by a number of authors, (3, 4) and compilations of measured and calculated frequencies have been made, calculations of the absorption coefficients corresponding to these transitions are not available. In order to obtain this information, a computer program was written to calculate both the frequencies and absorption coefficients. Since the results may be of interest to those studying the spectrum of SO_2, they are presented here.

In the first portion of the paper the method of calculation is described, and the results obtained are presented in table II. In the latter part, the calculated absorption coefficients are compared to existing experimental measurements (5) over the frequency range 26-40 GHz and to new measurements in the vicinity of 70 GHz. The experimental apparatus and techniques used in making these measurements are also described.

I. Calculations

A. Calculation of the Energy Levels

The common isotope, $^{32}S^{16}O_2$, of sulfur dioxide in its ground vibrational state is an asymmetric top with molecular symmetry C_{2v} and a dipole moment μ_b lying along the axis of intermediate moment of inertia. The rotational states can be identified by the quantum numbers $J(K_p, K_o)$ where J is the total rotational quantum number and K_p and K_o are pseudo-quantum numbers describing the projection of J on the symmetry axis for the limiting prolate and oblate symmetric tops, respectively. Because of the molecular symmetry and the zero nuclear spin of ^{16}O, only states of the form (e,e) and (o,o) are allowed, where e and o specify the parity of the pseudo quantum numbers. The only permitted dipole transitions are $(e,e) \leftrightarrow (o,o)$ with $\Delta J = 0, \pm 1$.

Because of contributions due to centrifugal distortion, the rigid rotor approximation is inadequate to describe the rotational energy levels except for very low J values. In order to account for distortion effects, the rotational Hamiltonian can be expressed in the form $H = H_2 + H_4 + H_6 + \ldots$ where the subscripts denote angular momentum operators of the nth power. For a rigid rotor, only terms of H_2 are used.

The theory of centrifugal distortion has been considered by Kivelson and Wilson (6) and by Watson (7). The Kivelson-Wilson formalism has the advantage that the parameters used

to describe the quartic Hamiltonian, $H_2 + H_4$, can be related directly to the physical properties of the molecule such as the moments of inertia and the vibrational force constants. However, Watson has shown that the parameters obtained in this way are not all independent, and hence cannot be used to obtain a unique fit to the observed rotational spectrum. By means of an appropriate similarity transformation, Watson has obtained a set of independent parameters which can, however, be used to fit the experimental data.

The microwave spectrum of $^{32}S^{16}O_2$ has been measured and analyzed by a number of authors (3, 4). The most extensive measurements are due to Steenbeckeliers (3), who interpreted them in terms of the Watson formalism. Kirchhoff (8) has reviewed the Watson treatment in detail, and has obtained from the data of Steenbeckeliers and others a 16-parameter fit to the spectrum, including terms of the Hamiltonian up to H_6. These parameters have recently been revised by Lovas (9), and in this form were used in the present calculation. For the sake of completeness they are reproduced in table I.

A computer program was written to set up and diagonalize the rotational Hamiltonian matrices for each of the transitions permitted by the dipole selection rules. The form of the Hamiltonian chosen for $H_2 + H_4$ was identical to that used by Kirchhoff (8), and the necessary matrix elements were taken from his appendix A. The Wang-transformed prolate symmetric

rotor basis set was used, and the resulting sub-matrices obtained for each J value were diagonalized by computer. The contributions to the energy due to H_6 were obtained by first order perturbation theory using eigenfunctions of $H_2 + H_4$.

B. Calculation of the Absorption Coefficients

At the pressures normally employed in microwave spectroscopy, the unsaturated lineshape is approximately Lorentzian and the absorption coefficient has the form (10)

$$\gamma(\nu) = \frac{CN\nu^2(\Delta\nu)}{(\nu-\nu_o)^2 + (\Delta\nu)^2}, \qquad (1)$$

where N is the number of molecules per cm^3 of the absorbing gas and ν_o is the resonant frequency. In the pressure broadening regime (approximately 0.01-10 Torr), the linewidth $\Delta\nu$ is proportional to the pressure. Since the concentration N is also proportional to the pressure, the peak absorption at resonance $\gamma(\nu_o)$ is pressure independent and is therefore a convenient parameter to characterize the magnitude of absorption.

Under these conditions the peak absorption is given by (10)

$$\gamma_{max} = \frac{8\pi^2\nu_o^2 f_v}{3ckT} \frac{(2J+1)|\mu_{ij}|^2}{Q_r} \left(\frac{N}{\Delta\nu}\right) e^{-W/kT}, \qquad (2)$$

where $|\mu_{ij}|$ is the magnitude of the dipole matrix element for the transition considered, W is the energy of the lower

state, T is the absolute temperature, and f_v is the fraction of molecules in the ground vibrational state. Using the known fundamental vibrational frequencies (11) of $^{32}S^{16}O_2$, the value $f_v = 0.917$ was obtained for T = 293K. For the rotational partition function Q_r, the expression (10)

$$Q_r = \frac{1}{\sigma}\sqrt{\frac{\pi}{ABC}\left(\frac{kT}{h}\right)^3} \qquad (3)$$

was used. For $^{32}S^{16}O_2$ the symmetry number, $\sigma = 2$ and A,B,C are the rotational constants. The ratio $N/\Delta\nu$ can be evaluated once the linewidth is known at a given pressure. If $(\Delta\nu)_1$, the linewidth in MHz at one torr and 293K is specified, $N/\Delta\nu = 3.2957 \times 10^{10}/(\Delta\nu)_1$.

The quantity $(2J+1)|\mu_{ij}|^2$ can be expressed in terms of the line strength (10) for the transition defined as

$$S_{ij} = \frac{(2J+1)|\mu_{ij}|^2}{\mu^2} \quad , \qquad (4)$$

where $\mu = 1.634D$ is the dipole moment (12) for SO_2 ($1D = 10^{-18}$ esu). Line strengths for each transition were calculated using the direction cosine matrix elements derived by Schwendeman (13) and the wave functions obtained by diagonalizing the energy matrices.

C. Results

Calculated frequencies and absorption coefficients are given in table II for all transitions up to J=50 having absorption coefficients greater than 10^{-10} cm^{-1} and frequencies

less than 200 GHz. Also given are the transition line strengths and the upper and lower state energies in units of cm^{-1}.

The calculated frequencies were compared to the available measured data (3, 4), and the average (RMS) deviation was found to be about 0.05 MHz. The largest deviation noted was about 0.2 MHz.

In order to calculate the absorption coefficients, it was necessary to assume a value for the linewidth parameter, $(\Delta\nu)_1$. Measurements and calculations (14) of the self-broadened linewidths for SO_2 have been reported for a limited number of transitions. However, in view of the uncertainty of these results and the lack of data for the majority of cases, an average linewidth of 16 MHz/torr was assumed, independent of the transition involved, although the linewidths are known to vary by as much as ±30%. If the actual linewidth for a given transition is known, however, the calculated absorption coefficient can be corrected by multiplying by the appropriate ratio.

In calculating the absorption coefficients a room temperature value of 293K (20°C) was assumed. Corrected coefficients for other temperatures can be easily determined from equation (2) with the use of the line strengths and energy levels given in table II. Since the abundance

of $^{32}S^{16}O_2$ in naturally occurring sulfur dioxide is about 94.5%, the coefficients in table II should be multiplied by 0.945 to obtain the absorption in a normal sample.

II. Comparison with Experimental Measurements

The measurement of intensities of microwave absorption lines by conventional spectrometers is known to be subject to large errors. With the widely used Stark-waveguide spectrometer, accuracies of absolute measurements (15) are rarely better than about 25 or 30%. For strongly absorbing substances, methods (16) have been introduced for making absolute measurements accurate to within about 5%. More recently, microwave spectrometers said to be capable of measuring the intensities of weaker absorption lines to within 5% have been described (17).

A. Measurements between 26 and 40 GHz

Measurements of the microwave spectrum of SO_2 have recently been made by White (5), using a commercial computerized spectrometer. This instrument incorporated a calibration arm which permitted the sample cell absorption to be simulated by a precision attenuator and a diode switch connected to the Stark modulator. With this spectrometer it was possible to measure automatically not only the frequencies but also the linewidths and absorption coefficients.

In table III a comparison is shown of White's measurements and the calculated peak absorption coefficients for a number of transitions of $^{32}S^{16}O_2$. The measurements were made at a temperature of 293 K and a pressure of 15 mtorr. A microwave power level of about 0.02 mwatt was used in order to minimize saturation effects. The uncertainties for the experimental linewidth parameters and absorption coefficients were estimated by the author (5) to be about ±10%. The calculated absorption coefficients were adjusted to correspond to the observed linewidths as described above.

As can be seen from the table, the agreement between the calculated and observed absorption coefficients is quite good, considering the uncertainties involved. However, it should be noted that the calculated absorption coefficients are, on the average, about 10% smaller than the measured values. The reason for this apparent bias is not entirely understood. The measured linewidths have not been corrected for contributions arising from the Doppler effect or for any instrumental effects such as modulation or saturation broadening, and may be slightly larger than their true values (18). Independent measurements of the linewidths for a few of the transitions given in table III have been reported (14) and were found to be narrower than the present values.

B. Measurements at 70 GHz

Additional measurements of some of the stronger transitions of SO_2 in the vicinity of 70 GHz were made in this laboratory. A transmission cavity type of spectrometer employing a semi-confocal Fabry-Perot interferometer (19) was used. The cavity consisted of two highly polished mirrors approximately 5 cm in diameter, silver plated and gold flashed. The concave mirror was spherical with a radius of curvature of 14.86 cm, and could be translated along its axis for tuning purposes by means of a micrometer drive of the type used in microscopes. The flat mirror contained two coupling holes about a centimeter apart, behind which the machined ends of the waveguides could be positioned. With this arrangement (20) it was possible to control the amount of coupling and the quality factor Q of the cavity by adjusting the insertion depth of the waveguides. The cavity was operated in the fundamental TEM_{ooq} mode with a mirror separation approximately equal to half the mirror radius. At 69 GHz the number of half wavelengths q between the mirrors was equal to 34. The loaded Q of the cavity was about 25,000 and the transmission loss at resonance was about 18 dB.

Microwave power was supplied by an OKI 70V10A klystron mounted in a large oil bath for cooling and thermal stabilization. A Baytron wafer-type crystal detector was used

to monitor the output of the transmission cavity. The sensitivity of this detector was measured, using a TRG wet calorimeter, and found to be about 0.3 mV/μW when terminated in a one megohm load. The microwave frequencies were measured by zero-beating the 7th harmonic of a tunable, stabilized, X-band source with the OKI V-band klystron output. A counter directly measured the X-band source frequency. In addition, a diode modulator was used to provide a "fence" of marker frequencies on either side of the primary reference frequency.

The cavity was mounted in a stainless steel chamber attached to a 6" diffusion pump vacuum system. A gas handling system consisting of a pressure regulator, a needle valve to bleed gas into the chamber, and a bypass valve connected to the vacuum pump was employed. The chamber could either be filled statically to a given pressure or maintained under flowing conditions at any desired pressure by suitable adjustment of the valves. The latter configuration was preferred because it enabled the pressure to be changed rapidly from vacuum to the desired value in a reproducible fashion, simply by opening or closing a small bellows valve in series with the needle valve. The gas pressure in the chamber was measured with a calibrated capacitance manometer, and the gas temperature was determined by thermocouples attached to the chamber.

The absorption coefficients were measured by employing the relationship (16, 21)

$$\gamma = \frac{2\pi\nu_o}{c}\left(\frac{1}{Q_1} - \frac{1}{Q_o}\right) = \frac{2\pi\nu_o}{cQ_o}\left[\sqrt{\frac{P_o}{P_1}} - 1\right], \qquad (5)$$

where ν_o is the frequency of the transition, c is the velocity of light, Q_o is the loaded Q of the cavity without the gas absorption, and Q_1 is the Q with the gas present. P_1 and P_o represent respectively the peak output power of the cavity with and without the gas. The second form of Eq. (5) follows from the fact that, for a loosely coupled detector, the detected power varies as Q^2.

The Q of the empty cavity was measured by superimposing the frequency markers from the modulated X-band source on the 3dB-down points of the cavity response curve. The half-power points were established using a precision attenuator. It was found that the Q values obtained in this way were reproducible to within 3%, although the variations over a large frequency range and from day to day were larger. The Q value measurements were repeated at a number of points over the frequency range encompassing the absorption line and were found to be constant to within the above precision.

The SO_2 gas, Matheson anhydrous grade with a stated purity of 99.98%, was then introduced into the cavity using the flowing system described above. A pressure of approximately 300 mtorr was used for all the absorption lines measured. After measuring the peak response of the cavity, the gas was quickly pumped out of the chamber and the output power restored to the same value by means of the precision attenuator. This process was then repeated at a number of frequencies over the width of each absorption line, and the absorption coefficients were calculated from Eq. (5). The resulting plot of absorption coefficient versus frequency was then used to obtain the peak absorption coefficient, $\gamma_{obs.}$ and the linewidth parameter, $(\Delta\nu)_1$. The observed and calculated peak absorption coefficients for the transitions measured are shown in table IV. As in table III the calculated absorption coefficients were obtained by using the measured linewidth parameters and the temperatures shown in the table.

In measuring the absorption coefficients, care was taken to avoid saturation. In each case the microwave power level was reduced until no further increase in peak absorption could be observed. The microwave power entering the cavity under these conditions was estimated to be about 100 μ watts from calorimeter data and a measurement of the input coupling coefficient. At this power level the amount of saturation expected was calculated to be no more than 3% for the 6(1,5)-6(0,6) transition, and less for the other transitions observed.

Each transition was measured several times to obtain an estimate of the reliability of the data, and the values obtained for the linewidth parameters and peak absorption coefficients were found to be consistent from run to run to within about 5%. As can be seen from table IV, the calculated and observed absorption coefficients are also in agreement within this precision. Calculated values (22) for the linewidth parameters of some of the transitions in table IV are available. These were found to be between 5 and 15% smaller than the values measured here. The only case for which a prior measurement of the linewidth parameter is available is the 1(1,1)-0(0,0) transition. The value obtained (14) in this case was 12 MHz/torr, about 14% smaller than the present value. The reason for this discrepancy is not completely clear, and further measurements are planned to determine whether instrumental effects such as transmission-line resonances or other errors could be responsible.

III. Summary

The frequencies and absorption coefficients for the rotational transitions of $^{32}S^{16}O_2$ were calculated for frequencies up to 200 GHz. The results are in good agreement with existing measurements in the frequency range from 26 to 40 GHz and with new measurements in the vicinity of 70 GHz. The peak absorption coefficient for the 6(1,5)-6(0,6) transition at 68.9 GHz was found to be a factor of ten

larger than any of the transitions below 40 GHz, and appears to be a good candidate for a sensitive detector of SO_2 at low concentrations.

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Table I

Watson Determinable Parameters for $^{32}S^{16}O_2$

Rotational Constants	
A(MHz)	60778.55529 ± 0.0056
B(MHz)	10317.91220 ± 0.0011
C(MHz)	8799.651056 ± 0.00093

Distortion Constants	
τ_{aaaa}(MHz)	-9.917148 ± 0.00022
τ_{bbbb}(kHz)	-40.04591 ± 0.0075
τ_{cccc}(kHz)	-12.82923 ± 0.0062
τ_1(kHz)	388.3076 ± 0.11
τ_2(kHz)	31.57071 ± 0.017
τ_3(kHz)[a]	727.839 ± 0.44
H_j(MHz)	$(0.13729 \pm 0.014) \times 10^{-7}$
H_{jk}(MHz)	$(0.11286 \pm 0.029) \times 10^{-6}$
H_{kj}(MHz)	$(-0.184810 \pm 0.00080) \times 10^{-4}$
H_k(MHz)	$(0.354211 \pm 0.00059) \times 10^{-3}$
h_j(MHz)	$(0.10146 \pm 0.0024) \times 10^{-7}$
h_{jk}(MHz)	$(0.49316 \pm 0.048) \times 10^{-6}$
h_k(MHz)	$(0.12411 \pm 0.015) \times 10^{-4}$

[a]The value of τ_3 is set using the planarity conditions[8] and is not a determinable parameter.

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Table II

SO_2 Pure Rotational State Transitions

Transition Upper State $J(K_p,K_o)$	Transition Lower State $J(K_p,K_o)$	Calculated Frequency MHz	Absorption Coefficient cm^{-1}	Line Strength	Energy Levels Upper State cm^{-1}	Energy Levels Lower State cm^{-1}
39(7,33)	38(8,30)	521.431	1.798E-09	6.0229	583.185	583.167
27(2,26)	26(3,23)	2838.924	4.269E-08	0.9116	243.898	243.803
43(9,35)	44(8,36)	3045.788	3.157E-08	6.7961	743.136	743.035
19(3,17)	18(4,14)	4027.080	4.543E-07	2.8501	136.917	136.782
38(4,34)	39(3,37)	4195.719	2.965E-08	1.0690	509.729	509.589
11(3, 9)	12(2,10)	4546.071	5.623E-07	1.8746	57.549	57.398
29(5,25)	28(6,22)	6837.403	8.305E-07	4.4710	321.458	321.230
34(6,28)	33(7,27)	6848.427	5.397E-07	5.2544	442.748	442.520
15(2,14)	14(3,11)	7169.597	1.334E-06	2.0252	82.937	82.698
48(10,38)	49(9,41)	7503.519	8.854E-08	7.5687	922.405	922.154
12(2,10)	13(1,13)	8420.277	8.062E-07	0.7824	57.398	57.117
27(6,22)	28(5,23)	8911.143	1.480E-06	4.2889	303.254	302.957
18(3,15)	17(4,14)	9403.178	2.566E-06	2.7892	125.498	125.184
10(2, 8)	11(1,11)	11788.887	1.979E-06	0.9096	42.347	41.953
22(5,17)	23(4,20)	12132.491	3.633E-06	3.4957	204.543	204.139
1(1, 1)	2(0, 2)	12256.593	1.496E-06	0.5224	2.321	1.912
50(9,41)	49(10,40)	13599.492	2.555E-07	7.7680	954.268	953.814
14(2,12)	15(1,15)	14587.756	1.763E-06	0.6215	75.150	74.663
32(7,25)	33(6,28)	16681.036	3.426E-06	5.0525	421.351	420.795
45(8,38)	44(9,35)	17539.857	9.374E-07	6.9930	771.939	771.354
37(8,30)	38(7,31)	19637.091	2.788E-06	5.8251	558.793	558.138
12(3, 9)	13(2,12)	20335.437	1.060E-05	1.8292	65.306	64.627
24(4,20)	23(5,19)	22482.530	1.235E-05	3.7275	220.036	219.286
40(7,33)	39(8,32)	23034.772	3.205E-06	6.2209	608.955	608.186
5(2, 4)	6(1, 5)	23414.284	9.300E-06	0.9520	16.395	15.614
21(5,17)	22(4,18)	24039.688	1.457E-05	3.3243	190.419	189.617
8(2, 6)	9(1, 9)	24083.495	9.043E-06	0.9353	29.988	29.185
42(9,33)	43(8,36)	24319.697	2.244E-06	6.5952	715.566	714.755
49(4,46)	48(5,43)	24915.569	3.198E-07	1.4106	808.146	807.315
35(6,30)	34(7,27)	25049.453	6.718E-06	5.4415	465.180	464.345
8(1, 7)	7(2, 6)	25392.777	1.768E-05	1.6092	25.518	24.671
25(4,22)	24(5,19)	26776.598	1.678E-05	3.8508	235.619	234.726
25(2,24)	24(3,21)	27932.453	6.191E-06	1.1575	211.076	210.144
47(10,38)	48(9,39)	28179.370	1.419E-06	7.3675	891.641	890.701
17(2,16)	16(3,13)	28858.023	2.005E-05	2.0726	103.712	102.750
4(0, 4)	3(1, 3)	29321.309	2.686E-05	1.6671	6.360	5.382

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0 0 0 0 4 2 0 2 7 4 5

Table II (continued)

Transition Upper State $J(K_p,K_o)$	Transition Lower State $J(K_p,K_o)$	Calculated Frequency MHz	Absorption Coefficient cm^{-1}	Line Strength	Energy Levels Upper State cm^{-1}	Energy Levels Lower State cm^{-1}
16(2,14)	17(1,17)	30205.535	5.231E-06	0.4742	95.589	94.581
28(3,25)	29(2,28)	31089.905	3.401E-06	0.7200	280.123	279.086
16(4,12)	17(3,15)	31922.318	2.824E-05	2.5117	114.309	113.244
26(6,20)	27(5,23)	34097.780	2.254E-05	4.0804	285.940	284.803
31(7,25)	32(6,26)	36065.305	1.707E-05	4.8540	400.825	399.622
30(5,25)	29(6,24)	36338.109	2.241E-05	4.6803	341.048	339.835
21(3,19)	20(4,16)	37351.820	3.769E-05	3.1088	163.122	161.877
15(4,12)	16(3,13)	38518.290	4.069E-05	2.3609	104.035	102.750
37(3,35)	36(4,32)	38909.681	3.994E-06	1.3139	461.494	460.196
46(8,38)	45(9,37)	39446.897	4.230E-06	7.1887	801.533	800.217
36(8,28)	37(7,31)	41177.468	1.334E-05	5.6219	535.068	533.695
41(7,35)	40(8,32)	42680.027	9.994E-06	6.4101	635.281	633.858
19(2,18)	18(3,15)	43016.298	3.777E-05	1.9650	126.933	125.498
23(2,22)	22(3,19)	43178.212	2.150E-05	1.4450	180.632	179.191
6(2, 4)	7(1, 7)	44052.893	2.750E-05	0.8080	20.294	18.825
41(9,33)	42(8,34)	44875.915	8.481E-06	6.3925	688.642	687.145
31(5,27)	30(6,24)	47660.655	3.623E-05	4.8351	360.710	359.120
14(2,12)	13(3,11)	47913.372	7.373E-05	2.3956	75.150	73.551
21(2,20)	20(3,17)	48120.468	3.683E-05	1.7350	152.579	150.973
46(10,36)	47(9,39)	48958.240	4.844E-06	7.1637	861.522	859.889
36(6,30)	35(7,29)	51185.245	2.604E-05	5.6398	488.515	486.808
20(5,15)	21(4,18)	51736.716	6.761E-05	3.1043	176.962	175.236
10(3, 7)	11(2,10)	52051.803	6.224E-05	1.5173	50.538	48.802
25(6,20)	26(5,21)	52188.539	5.468E-05	3.8819	269.265	267.525
9(3, 7)	10(2, 8)	53015.296	6.135E-05	1.3968	44.115	42.347
2(1, 1)	2(0, 2)	53528.858	1.345E-04	2.4627	3.697	1.912
40(4,36)	41(3,39)	54139.130	3.197E-06	0.8869	561.844	560.038
18(2,16)	19(1,19)	54633.575	1.161E-05	0.3589	118.685	116.862
30(7,23)	31(6,26)	58042.664	4.684E-05	4.6475	380.950	379.014
4(1, 3)	4(0, 4)	59224.862	2.746E-04	4.1981	8.336	6.360
47(8,40)	46(9,37)	59883.412	8.655E-06	7.3787	831.728	829.731
35(8,28)	36(7,29)	61489.860	3.222E-05	5.4174	511.989	509.938
20(3,17)	19(4,16)	61636.159	1.134E-04	3.2231	150.973	148.917
27(4,24)	26(5,21)	64277.225	8.873E-05	4.1525	269.669	267.525
40(9,31)	41(8,34)	65714.082	2.009E-05	6.1869	662.364	660.172
23(3,21)	22(4,18)	66724.920	1.099E-04	3.2550	191.842	189.617
42(7,35)	41(8,34)	66761.059	2.213E-05	6.6029	662.399	660.172
37(6,32)	36(7,29)	67011.291	4.103E-05	5.8099	512.173	509.938
19(5,15)	20(4,16)	67848.712	1.163E-04	2.9072	164.140	161.877

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Table II (continued)

Transition Upper State $J(K_p,K_o)$	Transition Lower State $J(K_p,K_o)$	Calculated Frequency MHz	Absorption Coefficient cm^{-1}	Line Strength	Energy Levels Upper State cm^{-1}	Energy Levels Lower State cm^{-1}
6(1, 5)	6(0, 6)	68972.145	4.751E-04	5.5417	15.614	13.313
14(4,10)	15(3,13)	69464.143	1.253E-04	2.1215	94.435	92.118
45(10,36)	46(9,37)	69480.424	1.099E-05	6.9580	832.048	829.731
1(1, 1)	0(0, 0)	69575.918	9.313E-05	1.0000	2.321	0.000
3(2, 2)	4(1, 3)	69653.602	3.631E-05	0.4052	10.659	8.336
4(2, 2)	5(1, 5)	70134.391	4.738E-05	0.5281	13.226	10.886
30(3,27)	31(2,30)	72437.264	1.235E-05	0.5790	319.048	316.632
26(4,22)	25(5,21)	72668.072	1.222E-04	4.1188	253.170	250.746
6(0, 6)	5(1, 5)	72758.210	2.906E-04	3.0104	13.313	10.886
35(3,33)	34(4,30)	73430.451	2.221E-05	1.6293	415.761	413.312
24(6,18)	25(5,21)	74866.567	1.155E-04	3.6707	253.243	250.746
10(1, 9)	9(2, 8)	76412.116	2.269E-04	2.4040	38.027	35.478
47(4,44)	46(5,41)	76539.860	4.933E-06	1.6945	747.157	744.604
29(7,23)	30(6,24)	77926.741	8.896E-05	4.4411	361.720	359.120
34(8,26)	35(7,29)	82409.535	6.234E-05	5.2095	489.557	486.808
48(8,40)	47(9,39)	82752.788	1.462E-05	7.5688	862.649	859.889
13(4,10)	14(3,11)	82952.019	1.700E-04	1.9277	85.465	82.698
8(1, 7)	8(0, 8)	83688.071	7.685E-04	6.3767	25.518	22.727
32(5,27)	31(6,26)	84320.923	1.075E-04	5.0545	381.827	379.014
43(7,37)	42(8,34)	85246.955	3.246E-05	6.7804	689.989	687.145
39(9,31)	40(8,32)	86153.727	3.799E-05	5.9795	636.732	633.858
8(3, 5)	9(2, 8)	86639.137	1.372E-04	1.1309	38.368	35.478
20(2,18)	21(1,21)	86828.918	1.996E-05	0.2757	144.397	141.501
33(5,29)	32(6,26)	87926.348	1.079E-04	5.1623	402.555	399.622
44(10,34)	45(9,37)	90005.081	2.068E-05	6.7503	803.220	800.217
25(3,23)	24(4,20)	90548.220	1.744E-04	3.2581	223.056	220.036
18(5,13)	19(4,16)	91550.522	2.087E-04	2.6892	151.971	148.917
49(11,39)	50(10,40)	93641.777	1.002E-05	7.5227	988.993	985.870
23(6,18)	24(5,19)	94064.767	1.861E-04	3.4621	237.864	234.726
38(6,32)	37(7,31)	97466.399	7.988E-05	6.0079	536.946	533.695
7(3, 5)	8(2, 6)	97702.389	1.490E-04	0.9403	33.247	29.988
33(3,31)	32(4,28)	97994.155	6.056E-05	2.0083	372.404	369.135
28(7,21)	29(6,24)	98976.324	1.503E-04	4.2301	343.137	339.835
29(4,26)	28(5,23)	99392.605	1.879E-04	4.3772	306.272	302.957
2(2, 0)	3(1, 3)	100878.119	3.070E-05	0.1610	8.747	5.382
33(8,26)	34(7,27)	102690.045	1.037E-04	4.9999	467.770	464.345
49(8,42)	48(9,39)	102707.110	1.982E-05	7.7500	894.127	890.701
3(1, 3)	2(0, 2)	104029.398	4.156E-04	2.0148	5.382	1.912
16(2,14)	15(3,13)	104033.541	3.968E-04	2.9960	95.589	92.118
10(1, 9)	10(0,10)	104239.272	1.182E-03	6.6996	38.027	34.549

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0 0 0 0 4 2 0 2 7 4 6

Table II (continued)

Transition Upper State $J(K_p,K_o)$	Transition Lower State $J(K_p,K_o)$	Calculated Frequency MHz	Absorption Coefficient cm^{-1}	Line Strength	Energy Levels Upper State cm^{-1}	Energy Levels Lower State cm^{-1}
38(9,29)	39(8,32)	106674.763	6.374E-05	5.7698	611.744	608.186
27(3,25)	26(4,22)	107060.307	1.974E-04	3.1035	256.741	253.170
12(4, 8)	13(3,11)	107843.549	2.653E-04	1.7011	77.149	73.551
42(4,38)	43(3,41)	108915.432	8.502E-06	0.7553	616.467	612.834
39(6,34)	38(7,31)	108955.965	9.065E-05	6.1514	561.773	558.138
17(5,13)	18(4,14)	109757.682	2.935E-04	2.4786	140.444	136.782
43(10,34)	44(9,35)	110363.756	3.471E-05	6.5409	775.035	771.354
31(3,29)	30(4,26)	111755.115	1.163E-04	2.4200	331.436	327.708
44(7,37)	43(8,36)	111875.496	5.018E-05	6.9690	718.487	714.755
48(11,37)	49(10,40)	113970.825	1.690E-05	7.3132	957.616	953.814
29(3,27)	28(4,24)	114565.473	1.715E-04	2.8074	292.875	289.053
22(6,16)	23(5,19)	115317.631	2.830E-04	3.2473	223.132	219.286
8(0, 8)	7(1, 7)	116980.408	1.104E-03	4.6013	22.727	18.825
22(3,19)	21(4,18)	118577.435	4.219E-04	3.6874	179.191	175.236
27(7,21)	28(6,22)	118994.267	2.260E-04	4.0180	325.199	321.230
32(3,29)	33(2,32)	119483.027	2.282E-05	0.4785	360.516	356.530
45(4,42)	44(5,39)	120023.415	1.981E-05	2.0607	688.523	684.520
6(3, 3)	7(2, 6)	123057.734	1.835E-04	0.7109	28.776	24.671
32(8,24)	33(7,27)	123194.663	1.591E-04	4.7878	446.629	442.520
11(4, 8)	12(3, 9)	124864.844	3.242E-04	1.4892	69.471	65.306
22(2,20)	23(1,23)	125427.214	2.885E-05	0.2180	172.676	168.492
37(9,29)	38(8,30)	126962.421	9.836E-05	5.5584	587.402	583.167
35(5,31)	34(6,28)	126980.819	1.918E-04	5.4380	446.984	442.748
50(8,42)	49(9,41)	127081.815	2.662E-05	7.9346	926.393	922.154
28(4,24)	27(5,23)	127428.272	3.478E-04	4.5075	289.053	284.803
45(7,39)	44(8,36)	128103.796	5.859E-05	7.1300	747.308	743.035
12(2,10)	12(1,11)	128605.086	2.428E-03	9.9022	57.398	53.108
12(1,11)	11(2,10)	129105.736	8.529E-04	3.3797	53.108	48.802
10(2, 8)	10(1, 9)	129514.783	2.086E-03	7.7914	42.347	38.027
42(10,32)	43(9,35)	130679.859	5.410E-05	6.3297	747.495	743.136
31(4,28)	30(5,25)	130859.558	2.775E-04	4.4960	345.413	341.048
12(1,11)	12(0,12)	131014.811	1.727E-03	6.6440	53.108	48.738
16(5,11)	17(4,14)	131274.959	4.051E-04	2.2595	129.563	125.184
14(2,12)	14(1,13)	132744.800	2.806E-03	11.7146	75.150	70.722
8(2, 6)	8(1, 7)	134004.802	1.735E-03	5.6922	29.988	25.518
47(11,37)	48(10,38)	134203.763	2.654E-05	7.1023	926.881	922.405
21(6,16)	22(5,17)	134943.377	3.891E-04	3.0325	209.045	204.543
5(1, 5)	4(0, 4)	135695.985	1.075E-03	3.1320	10.886	6.360
34(5,29)	33(6,28)	135963.134	2.438E-04	5.4126	425.330	420.795

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Table II (continued)

Transition Upper State $J(K_p,K_o)$	Transition Lower State $J(K_p,K_o)$	Calculated Frequency MHz	Absorption Coefficient cm^{-1}	Line Strength	Energy Levels Upper State cm^{-1}	Energy Levels Lower State cm^{-1}
5(3, 3)	6(2, 4)	139355.077	1.703E-04	0.5048	24.943	20.294
26(7,19)	27(6,22)	139474.534	3.211E-04	3.8032	307.907	303.254
6(2, 4)	6(1, 5)	140306.160	1.344E-03	3.8327	20.294	15.614
16(2,14)	16(1,15)	143057.045	3.270E-03	12.9707	95.589	90.817
31(8,24)	32(7,25)	143357.780	2.284E-04	4.5742	426.133	421.351
40(6,34)	39(7,33)	146393.784	1.495E-04	6.3570	588.068	583.185
10(4, 6)	11(3, 9)	146550.129	3.949E-04	1.2678	62.438	57.549
4(2, 2)	4(1, 3)	146605.515	9.020E-04	2.2725	13.226	8.336
36(9,27)	37(8,30)	147239.172	1.434E-04	5.3452	563.705	558.793
15(5,11)	16(4,12)	150381.179	5.070E-04	2.0425	119.325	114.309
41(6,36)	40(7,33)	150487.014	1.414E-04	6.4573	613.974	608.955
41(10,32)	42(9,33)	150878.656	7.979E-05	6.1170	720.599	715.566
2(2, 0)	2(1, 1)	151378.659	3.769E-04	0.8707	8.747	3.697
43(4,40)	42(5,37)	153677.165	5.239E-05	2.5077	632.257	627.131
46(11,35)	47(10,38)	154373.232	3.963E-05	6.8899	896.790	891.641
20(6,14)	21(5,17)	155389.715	5.133E-04	2.8148	195.602	190.419
33(4,30)	32(5,27)	157135.414	3.263E-04	4.4790	387.068	381.827
3(2, 2)	3(1, 3)	158199.773	6.763E-04	1.4423	10.659	5.382
46(7,39)	45(8,38)	158845.046	8.021E-05	7.3172	777.238	771.939
25(7,19)	26(6,20)	159447.971	4.309E-04	3.5872	291.259	285.940
18(2,16)	18(1,17)	160342.940	3.846E-03	13.5645	118.685	113.336
4(3, 1)	5(2, 4)	160543.066	1.385E-04	0.3028	21.750	16.395
10(0,10)	9(1, 9)	160827.792	2.773E-03	6.4303	34.549	29.185
18(2,16)	17(3,15)	163119.361	1.092E-03	3.7203	118.685	113.244
30(8,22)	31(7,25)	163567.624	3.134E-04	4.3588	406.281	400.825
14(1,13)	14(0,14)	163605.504	2.396E-03	6.4105	70.722	65.264
37(5,33)	36(6,30)	163924.886	2.649E-04	5.6418	493.983	488.515
9(4, 6)	10(3, 7)	165123.722	4.307E-04	1.0522	56.046	50.538
5(2, 4)	5(1, 5)	165144.638	1.222E-03	2.4563	16.395	10.886
7(1, 7)	6(0, 6)	165225.412	2.179E-03	4.4298	18.825	13.313
44(4,40)	45(3,43)	166387.011	1.325E-05	0.6613	673.522	667.972
35(9,27)	36(8,28)	167367.207	1.998E-04	5.1307	540.651	535.068
24(2,22)	25(1,25)	168789.993	3.711E-05	0.1789	203.463	197.833
34(3,31)	35(2,34)	170293.690	3.212E-05	0.4080	404.456	398.776
14(5, 9)	15(4,12)	170754.656	6.135E-04	1.8229	109.730	104.035
40(10,30)	41(9,33)	171017.868	1.129E-04	5.9030	694.346	688.642
47(7,41)	46(8,38)	171036.665	8.191E-05	7.4534	807.238	801.533
45(11,35)	46(10,36)	174463.722	5.686E-05	6.6762	867.342	861.522

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0 0 0 0 4 2 0 2 7 4 7

Table II (continued)

Transition Upper State $J(K_p,K_o)$	Transition Lower State $J(K_p,K_o)$	Calculated Frequency MHz	Absorption Coefficient cm^{-1}	Line Strength	Energy Levels Upper State cm^{-1}	Energy Levels Lower State cm^{-1}
19(6,14)	20(5,15)	175101.415	6.424E-04	2.5966	182.803	176.962
7(2, 6)	7(1, 7)	175275.702	1.780E-03	3.3035	24.671	18.825
41(4,38)	40(5,35)	176295.978	1.083E-04	3.0120	578.375	572.494
35(4,32)	34(5,29)	176466.426	3.195E-04	4.3049	431.216	425.330
3(3, 1)	4(2, 2)	179006.143	7.324E-05	0.1268	19.197	13.226
24(7,17)	25(6,20)	179560.985	5.571E-04	3.3695	275.255	269.265
24(3,21)	23(4,20)	180045.344	9.658E-04	4.2195	210.144	204.139
14(1,13)	13(2,12)	182706.004	2.144E-03	4.5841	70.722	64.627
29(8,22)	30(7,23)	183582.666	4.137E-04	4.1422	387.074	380.950
20(2,18)	20(1,19)	184969.807	4.532E-03	13.5736	144.397	138.228
8(4, 4)	9(3, 7)	185278.425	4.455E-04	0.8378	50.295	44.115
37(4,34)	36(5,31)	187055.576	2.641E-04	3.9750	477.832	471.593
39(4,36)	38(5,33)	187338.074	1.845E-04	3.5236	526.893	520.644
30(4,26)	29(5,25)	187370.361	6.849E-04	4.9153	327.708	321.458
34(9,25)	35(8,28)	187446.553	2.689E-04	4.9147	518.242	511.989
9(2, 8)	9(1, 9)	188654.948	2.374E-03	4.0012	35.478	29.185
13(5, 9)	14(4,10)	190148.713	7.020E-04	1.6046	100.778	94.435
43(6,38)	42(7,35)	191021.046	1.823E-04	6.7149	668.771	662.399
39(10,30)	40(9,31)	191066.911	1.545E-04	5.6877	668.737	662.364
36(5,31)	35(6,30)	192236.352	4.172E-04	5.7614	471.593	465.180
2(2, 0)	1(1, 1)	192650.924	1.043E-03	1.4776	8.747	2.321
9(1, 9)	8(0, 8)	193609.379	3.843E-03	5.9573	29.185	22.727
44(11,33)	45(10,36)	194491.501	7.905E-05	6.4614	838.536	832.048
18(6,12)	19(5,15)	195080.384	7.774E-04	2.3774	170.647	164.140
22(3,19)	22(2,20)	195320.394	5.551E-03	17.6592	179.191	172.676
20(3,17)	20(2,18)	197142.031	5.669E-03	15.4061	150.973	144.397
39(5,35)	38(6,32)	197585.500	3.091E-04	5.7480	543.537	536.946
49(12,38)	50(11,39)	197709.529	3.617E-05	7.2361	1027.609	1021.014
42(6,36)	41(7,35)	198847.984	2.247E-04	6.6872	641.914	635.281
23(7,17)	24(6,18)	199415.906	6.952E-04	3.1510	259.895	253.243

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Table III

Calculated and Observed Absorption Coefficients for SO_2

Transition	Frequency MHz	$(\Delta\nu)_{1,obs.}$ MHz/torr	$\gamma_{obs.}$ cm^{-1}	$\gamma_{calc.}$ cm^{-1}
25(4,22) - 24(5,19)	26776.59	19	1.6×10^{-5}	1.4×10^{-5}
25(2,24) - 24(3,21)	27932.42	18	5.4×10^{-6}	5.3×10^{-6}
17(2,16) - 16(3,13)	28858.02	18	1.8×10^{-5}	1.7×10^{-5}
4(0, 4) - 3(1, 3)	29321.33	13	3.2×10^{-5}	3.2×10^{-5}
16(2,14) - 17(1,17)	30205.55	18	4.9×10^{-6}	4.4×10^{-6}
28(3,25) - 29(2,28)	31089.92	19	3.0×10^{-6}	2.7×10^{-6}
16(4,12) - 17(3,15)	31922.28	20	2.5×10^{-6}	2.1×10^{-6}
26(6,20) - 27(5,23)	34097.75	18	2.1×10^{-5}	1.9×10^{-5}
31(7,25) - 32(6,26)	36065.28	17	1.7×10^{-5}	1.5×10^{-5}
30(5,25) - 29(6,24)	36338.10	18	2.0×10^{-5}	1.9×10^{-5}
21(3,19) - 20(4,16)	37351.81	18	3.2×10^{-5}	3.1×10^{-5}
15(4,12) - 16(3,13)	38518.22	19	3.7×10^{-5}	3.3×10^{-5}
46(8,38) - 45(9,37)	39447.01	16	4.8×10^{-6}	4.1×10^{-6}

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Table IV

Calculated and Observed Absorption Coefficients for SO_2

Transition	Frequency MHz	Temp. °K	$(\Delta\nu)_{1,obs.}$ MHz/torr	$\gamma_{obs.}$ cm^{-1}	$\gamma_{calc.}$ cm^{-1}
19(5,15) - 20(4,16)	67848.7	297	18	9.4×10^{-5}	9.5×10^{-5}
6(1, 5) - 6(0, 6)	68972.2	298	15	4.5×10^{-4}	4.6×10^{-4}
14(4,10) - 15(3,13)	69464.1	297	19	1.0×10^{-4}	9.7×10^{-5}
1(1, 1) - 0(0, 0)	69575.9	297	14	9.2×10^{-5}	9.0×10^{-5}
26(4,22) - 25(5,21)	72668.1	298	19	9.6×10^{-5}	9.2×10^{-5}
6(0, 6) - 5(1, 5)	72758.2	300	14	2.7×10^{-5}	2.8×10^{-5}

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