

Peak Absorption Coefficients of Microwave Absorption Lines of Carbonyl Sulphide

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Peak absorption coefficients α_{\max} for the $J = 1 \leftarrow 0$, $J = 2 \leftarrow 1$ and $J = 3 \leftarrow 2$ rotational transitions in carbonyl sulphide have been calculated for the different isotopic molecular species in natural abundance and in each case for a range of vibrational states. The results are tabulated for convenience both in order of values of α_{\max} and in order of transition frequencies. Calculations have also been made, on a less extensive basis, for transitions from $J = 4 \leftarrow 3$ to $J = 25 \leftarrow 24$, and peak absorption coefficients have been tabulated, in order of values of α_{\max} , for each of these transitions. The tables provide a frequency coverage of approximately 10 to 300 GHz. Comparison with available experimental results shows satisfactory agreement.

Key words: absorption coefficients; carbonyl sulphide; intensities; microwave transitions; rotational transitions.

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1. Introduction

Carbonyl sulphide absorption lines have long been used as standards to monitor the sensitivities of microwave spectrometers. During some recent work employing a DECLAB 11-03 computer to increase sensitivity of a Hewlett-Packard 8460A microwave spectrometer the sensitivity of a spectrometer was investigated systematically by starting with the line belonging to the vibrational ground state $J = 3 \leftarrow 2$ transition in $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ at 33359.7 MHz ($\alpha_{\max} = 1.23 \times 10^{-8} \text{ cm}^{-1}$) and recording progressively weaker lines in the spectrum. In the course of the work it was noted with some surprise that no systematic tabulations of intensities of carbonyl sulphide absorption lines are

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available. The present paper aims to remedy this defect by giving tables of peak absorption coefficients which have been prepared for the purpose.

Calculations have been made for the $J = 1 \leftarrow 0$, $J = 2 \leftarrow 1$ and $J = 3 \leftarrow 2$ transitions and for ease of reference have been tabulated in sequence according to: (i) magnitude of α_{\max} (ii) frequency of the transition. In view of the increasing interest in higher frequency ranges calculations have also been made, though on a less extensive basis, for transitions from $J = 4 \leftarrow 3$ to $J = 25 \leftarrow 24$. For this group calculations have been made for the ground state and for the ℓ -doublets of the $\nu_2 = 1$ state (except for $^{18}\text{O}^{13}\text{C}^{34}\text{S}$ where the calculation is for the ground state only) and the results of these calculations are tabulated for each transition according to the magnitude of α_{\max} .

2. Peak Absorption Coefficients

Equations for line intensities have been given in a variety of ways and the opportunity is taken here to systematise equa-

tions for intensities and to set out an expression in a convenient form for computation. The peak absorption coefficient α_{\max} , for a rotational transition is given [1],¹ when expressed in the four-quantity system of equations, by

$$\alpha_{\max} = \frac{8\pi^2 n F_m \nu_0^2}{3ckT\Delta\nu} \left(\frac{1}{4\pi\epsilon_0} \right) \left(1 - \frac{1}{2} \frac{h\nu_0}{kT} \right) |\mu_{ij}|^2 \quad (1)$$

μ_{ij} is the transition moment, $\Delta\nu$ is the half width of the line measured between half intensity points (HWHH), ν_0 is the frequency of the transition, n is the number density of molecules, F_m is the fraction of molecules present in the lower state involved in the transition, and T is the temperature of the sample.

Two general points may be noted here. First, the number of molecules per unit volume is given by

$$n = \frac{pN_A a}{RT} \quad (2)$$

where N_A is the avogadro constant, p is the pressure, and a is the isotopic abundance for the molecular species involved.

Secondly, the dependence of the half width parameter $\Delta\nu$ on temperature and pressure may be expressed as

$$\Delta\nu = \frac{T^\theta}{T} \frac{p}{p^\theta} \Delta\nu^\theta \quad (3)$$

where $\Delta\nu^\theta$ is the standard half-width parameter at standard temperature T^θ and standard pressure p^θ . T^θ has generally been taken as 300 K, p^θ as 133 Pa (1 Torr) and the half-width parameter written as $(\Delta\nu)_1$.

Now for the calculation of F_m in the particular case of a linear molecule, the transition frequency can be related to the rotational constants by

$$\nu_0 = 2B(J+1) \quad (4)$$

the transition moment is related [2] to the dipole moment μ by

$$|\mu_{ij}|^2 = \mu^2 \left\{ \frac{(J+1)^2 - \ell^2}{(J+1)(2J+1)} \right\} \quad (5)$$

and

$$\begin{aligned} F_m &= F_v \frac{hB}{kT} (2J+1) e^{-hBJ(J+1)/kT} \\ &= F_v \frac{hB}{kT} (2J+1) e^{-hJ\nu_0/2kT} \end{aligned} \quad (6)$$

where F_v is the fraction of molecules in the vibrational state involved in the transition.

Substitution for n , $\Delta\nu$, ν_0^2 , $|\mu_{ij}|^2$ and F_m by means of Eqs. (2) and (6) in Eq. (1) yields

$$\begin{aligned} \alpha_{\max} &= \left\{ \frac{32\pi^2 h N_A}{3ck^2 R} \frac{p^\theta}{T^\theta} \frac{1}{4\pi\epsilon_0} \right\} \left\{ \frac{aF_v B^3 \mu^2}{T^2 \Delta\nu^\theta} (J+1) \right\} \\ &\times \{ (J+1)^2 - \ell^2 \} \\ &\times \left\{ 1 - \frac{1}{2} \frac{h\nu_0}{kT} \right\} e^{-hJ\nu_0/2kT} \end{aligned} \quad (7)$$

For purposes of computation it is convenient to use quantities in the form in which they are most commonly recorded, namely;

$$\nu_0/\text{GHz}, B/\text{GHz}, \mu/D^2, T/K, \Delta\nu^\theta/\text{MHz}$$

and

$$\alpha_{\max}/\text{cm}^{-1}$$

then,

$$\begin{aligned} \alpha_{\max} &= 0.039 30 \frac{aF_v B^3 \mu^2}{T^2 \Delta\nu^\theta} (J+1) \{ (J+1)^2 - \ell^2 \} \\ &\times \left\{ 1 - \frac{0.024 00 \nu_0}{T} \right\} e^{-0.024 00 J \nu_0 / T}. \end{aligned} \quad (8)$$

If the effects of anharmonicity on vibrational energy levels are neglected then the fraction F_v may be written as:

$$F_v = \frac{d_v e^{-\sum h\nu_i/kT}}{Q_v} \quad (9)$$

where the vibrational partition function is given by:

$$Q_v = \prod_i (1 - e^{-h\nu_i/kT})^{-d_i} \quad (10)$$

For the purposes of computation it is convenient to use wave numbers (ω_i/cm^{-1}) rather than frequencies ν_i . Then,

$$F_v = \frac{d_v e^{-1.439 \sum \nu_i \omega_i / T}}{Q_v} \quad (11)$$

and

$$Q_v = \prod_i (1 - e^{-1.439 \omega_i / T})^{-d_i} \quad (12)$$

2.1. Calculations

Peak absorption coefficients at 293 K calculated for lines belonging to $J=1\leftarrow 0$, $J=2\leftarrow 1$ and $J=3\leftarrow 2$ transitions for isotopic species in natural abundance and in each case for a range of vibrational states are given in tables 1 to 6. Natural abundance factors for the various isotopic species are given in table 8.

Harmonic wavenumbers ω_i for the various isotopic species of OCS have been calculated from the force constants of Morino and Nakagawa [8] viz.,

$$f_{RR}(\text{CS}) = 744.3 \pm 4.0,$$

$$f_{Rr} = 104.0 \pm 6.5,$$

$$f_{rr}(\text{CO}) = 1614 \pm 11 \text{ Nm}^{-1},$$

and

$$f_{\alpha\alpha} = (65.13 \pm 0.04) \times 10^{-20} \text{ J rad}^{-2}.$$

Electric dipole moments for all vibrational states with $\nu_2 = 0$, where ν_2 denotes the bending mode have been taken to be 0.715 29 D, [4] for all isotopic species. Dipole moments used for states with $\nu_2 = 1, 2, 3, 4$, and 5 were 0.704 33, [4] (0.693 18), 0.687 13 [5] (0.670 00) and (0.657 98) Debyes, respectively, where brackets denote estimates based on the known values.

The line width parameter $\Delta\nu^\theta$ is unfortunately not known as accurately as is desirable. Values reported for the $J=2\leftarrow 1$ transition [6] range from 6.0 to 6.5 MHz with the more reliable determinations [7] to [9] falling near 6.1 MHz. Measurements of $\Delta\nu^\theta$ for $J=1\leftarrow 0$ [10] and $J=3\leftarrow 2$ [11] transitions are also available. Theoretical calculations [12] predict an increase in $\Delta\nu^\theta$ with increasing J and consequently the values 6.05, 6.15, and 6.25 MHz for transitions with $J=0, 1$, and 2, respectively, which agree with most of the experimental measurements, have been assumed for the present calculations. All rotational constants and the reported transition frequencies have been taken from Maki's compilation [13] of the microwave spectral data available for OCS.

¹Figures in brackets indicate literature references at the end of this paper.

²D = 3.3356×10^{-30} C.m.

The results of the calculations of the peak absorption coefficients for the $J = 1 \leftarrow 0$, $J = 2 \leftarrow 1$ and $J = 3 \leftarrow 2$ transitions are tabulated in sequence in tables 1, 3, and 5 according to decreasing peak absorption coefficients, and in tables 2, 4, and 6 in decreasing order of transition frequencies. Quantum numbers v_1 , v_2 , and v_3 denoting the vibrational states refer to the CS stretching, the degenerate OCS angle bending and the CO stretching modes, respectively.

The calculations for higher J transitions given in table 7 called for further considerations about the calculation of frequencies and the choice of $\Delta\nu^\theta$. In order to calculate reasonably reliable frequencies, particularly for high J transitions, accurate values of B_v , D_v and q_v^ℓ are necessary. The values used in the calculations which are listed in table 9 have been taken from Maki's compilation supplemented by values from later papers [15] and [16]. Frequencies were calculated using:

$$\nu = [2B_v \pm \frac{1}{2}(v+1)(q_v^\ell + \delta J(J+1))](J+1) - 4D_v(J+1)(J+1)^2 - \ell^2 \quad (13)$$

where δ was set equal to zero in all cases except for $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ where

$$\delta = -4.272 \times 10^{-6}$$

was used [13]. No D_v values were available for the last four isotopic species in table 9, and in making the calculations for these species additivity in changes in D_v on isotopic substitution has been assumed. It is recognized that an estimate of D_v to ± 0.05 kHz results in a frequency uncertainty of ± 4 MHz for the highest J transition. It should generally be possible to identify the line concerned experimentally and in order to help in giving an indication of reliability of frequencies in table 8 the number of significant figures has been chosen so that uncertainty in the last quoted digit is probably less than 5.

Since the completion of the calculations some high J transitions have been reported [16] for some less abundant isotopic species of OCS. These results allow comparison for $J = 25 \leftarrow 24$ of $^{16}\text{O}^{13}\text{C}^{34}\text{S}$ for which the experimental value reported is 296150.275 MHz, which compares favorably with the calculated value in table 7. Moreover values reported for D_v of 1.237 869, 1.253 88, 1.257 85 kHz for the 00^0_0 , and the 01^1_0 states of $^{16}\text{O}^{13}\text{C}^{34}\text{S}$, and 1.077 88 kHz for the 00^0_0 state of $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ when compared with the values in table 9 agree well within the estimate of 0.05 kHz in the sample calculation given previously. Information on $\Delta\nu^\theta$ for the higher J transitions is sparse. Observed and calculated quantities which have been reported [11] up to the $J = 10 \leftarrow 9$ transition confirm that $\Delta\nu^\theta$ continues to increase with J , as expected from line-broadening theory, and leads to values of 6.33, 6.42, and 6.53 MHz Torr $^{-1}$ for $J = 3, 4$, and 5, respectively. The results also suggest that between $J = 6$ and 9 the variation is linear with J , values being given by $\Delta\nu^\theta = 5.895 + 0.124 J$. Accordingly we have used this expression for all transitions for $J > 6$.

There are two main factors which affect the reliability of the calculated peak absorption coefficients in tables 1 to 6. The first is uncertainty about the line width parameter already discussed. The second is the neglect of anharmonicity in the calculation of Boltzmann factors. An estimate has been made of this effect by calculating changes in the absorption coefficients resulting from a change of 10 cm^{-1} in ω_1 , ω_2 , and ω_3 in turn.

The effect on values of α_{max} for transitions in the ground vibrational state is found to be small ($< 1\%$) but values of α_{max} for transitions in vibrationally excited states are more sensitive and changes of up to about 5% were found for states with $v_i = 1$. Changes in α_{max} for states with more than one quantum of excitation will be correspondingly greater. This effect has to be combined with that resulting from uncertainty in $\Delta\nu^\theta$ which is about 2–3%. For higher J -transitions the uncertainty in $\Delta\nu^\theta$ already discussed is the main factor determining reliability of the peak absorption coefficients. However, even for the highest J transition ($J = 25 \leftarrow 24$) with a fairly generous error margin giving $9 \pm 2 \text{ MHz Torr}^{-1}$ for $\Delta\nu^\theta$, the resulting uncertainty in the peak absorption coefficients is about $\pm 20\%$. For many purposes in estimating sensitivities of spectrometers this is tolerable. In any case relative intensities for given transitions are reliable, and if $\Delta\nu^\theta$ becomes available or can be measured the correction is readily made. Thus many of the tabulated values of α are reliable to only two significant figures but three figures are given for convenience.

2.2. Comparison with Experiments

The sensitivity of the spectrometer was investigated systematically by starting with the $J = 3 \leftarrow 2$ line belonging to the ground vibrational state of $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ at 33359.7 MHz ($\alpha_{\text{max}} = 1.23 \times 10^{-8} \text{ cm}^{-1}$), and then recording progressively weaker lines, selected with the aid of tables 4 and 6, which were found to give reliable predictions of relative intensities of successive lines. The weakest line recorded was that for the $J = 3 \leftarrow 2$ transition in the (01^1_0) vibrational state of $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ with $\alpha_{\text{max}} = 8 \times 10^{-10} \text{ cm}^{-1}$. A recording of the line, which has not been previously reported is shown in figure 1, which reproduces an output trace obtained from digital storage acquired by the computer over a total scanning time of 34 minutes. The lower trace shows the result of digital smoothing and leads to a frequency measurement of 33402.80 MHz.

As a further comparison with experiment some of the calculated values of α_{max} are compared with available experimental measurements in table 10. The agreement is seen to be satisfactory considering the difference in halfwidths and temperatures between various experimental measurements and the present calculations. In fact, corrections for these differences would in most cases make the agreement even better.

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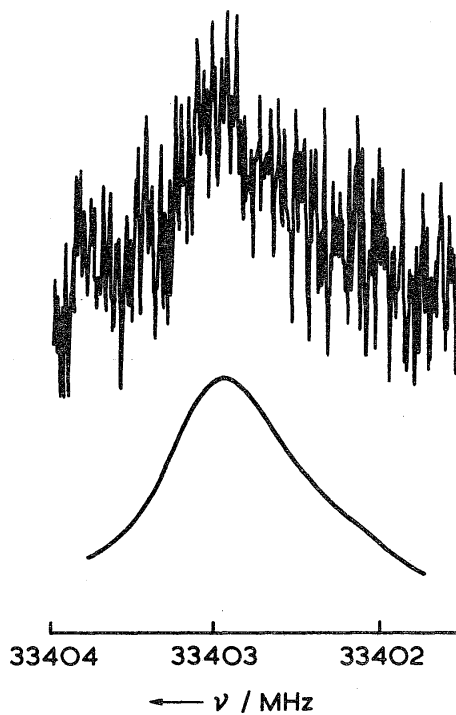


FIGURE 1. The $J = 3 \leftarrow 2$ rotational transition for the vibrational state (01^1_0) of $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ in natural abundance. The upper trace was obtained by digital recording over 512 data points with a total scanning time of 34 min and the lower trace shows the same line after digital smoothing.

TABLE 1. TRANSITIONS IN THE $J = 1 \leftarrow 0$ REGION OF OCS, ORDERED ACCORDING TO PEAK ABSORPTION COEFFICIENT IN NATURAL ABUNDANCE, AT 293 K

| | $\nu_1 \nu_2 \nu_3$ | ν/MHz | $\alpha_{\text{max}}/\text{cm}^{-1}$ |
|---|---------------------|------------------|--------------------------------------|
| $^{16}_0\text{C}^{12}_\text{C}^{32}_\text{S}$ | 00^0_0 | 12162.97 | 6.87×10^{-6} |
| $^{16}_0\text{C}^{12}_\text{C}^{34}_\text{S}$ | 00^0_0 | 11865.67 | 2.83×10^{-7} |
| $^{16}_0\text{C}^{12}_\text{C}^{32}_\text{S}$ | 10^0_0 | 12126.69 | 9.31×10^{-8} |
| $^{16}_0\text{C}^{13}_\text{C}^{32}_\text{S}$ | 00^0_0 | 12123.85 | 7.52×10^{-8} |
| $^{18}_0\text{C}^{12}_\text{C}^{32}_\text{S}$ | 00^0_0 | 11409.72 | 1.15×10^{-8} |
| $^{16}_0\text{C}^{12}_\text{C}^{34}_\text{S}$ | 10^0_0 | 11830.28 | 4.06×10^{-9} |
| $^{16}_0\text{C}^{13}_\text{C}^{34}_\text{S}$ | 00^0_0 | 11823.44 | 3.10×10^{-9} |
| $^{16}_0\text{C}^{12}_\text{C}^{32}_\text{S}$ | 20^0_0 | 12089.73 | 1.26×10^{-9} |
| $^{16}_0\text{C}^{13}_\text{C}^{32}_\text{S}$ | 10^0_0 | 12087.88 | 1.04×10^{-9} |
| $^{18}_0\text{C}^{12}_\text{C}^{34}_\text{S}$ | 00^0_0 | 11119.93 | 4.73×10^{-10} |
| $^{16}_0\text{C}^{12}_\text{C}^{32}_\text{S}$ | 00^0_1 | 12090.09 | 2.31×10^{-10} |
| $^{18}_0\text{C}^{12}_\text{C}^{32}_\text{S}$ | 10^0_0 | 11377.29 | 1.74×10^{-10} |
| $^{18}_0\text{C}^{13}_\text{C}^{32}_\text{S}$ | 00^0_0 | 11382.12 | 1.26×10^{-10} |
| $^{16}_0\text{C}^{12}_\text{C}^{34}_\text{S}$ | 20^0_0 | 11794.22 | 5.83×10^{-11} |
| $^{16}_0\text{C}^{13}_\text{C}^{34}_\text{S}$ | 10^0_0 | 11788.28 | 4.55×10^{-11} |
| $^{16}_0\text{C}^{13}_\text{C}^{32}_\text{S}$ | 20^0_0 | 12051.57 | 1.44×10^{-11} |

TABLE 2. TRANSITIONS IN THE $J = 1 \leftarrow 0$ REGION OF OCS, ORDERED ACCORDING TO FREQUENCY. PEAK ABSORPTION COEFFICIENTS ARE CALCULATED FOR NATURAL ABUNDANCE AND 293 K

| | $v_1 v_2 v_3$ | ν/MHz | $\alpha_{\text{max}}/\text{cm}^{-1}$ |
|---|-------------------|------------------|--------------------------------------|
| $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ | 00 ⁰ 0 | 11119.93 | 4.73×10^{-10} |
| $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 10 ⁰ 0 | 11377.29 | 1.74×10^{-10} |
| $^{18}\text{O}^{13}\text{C}^{32}\text{S}$ | 00 ⁰ 0 | 11382.12 | 1.26×10^{-10} |
| $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 00 ⁰ 0 | 11409.72 | 1.15×10^{-8} |
| $^{16}\text{O}^{13}\text{C}^{34}\text{S}$ | 10 ⁰ 0 | 11788.28 | 4.55×10^{-11} |
| $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | 20 ⁰ 0 | 11794.22 | 5.83×10^{-11} |
| $^{16}\text{O}^{13}\text{C}^{34}\text{S}$ | 00 ⁰ 0 | 11823.44 | 3.10×10^{-9} |
| $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | 10 ⁰ 0 | 11830.28 | 4.06×10^{-9} |
| $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | 00 ⁰ 0 | 11865.67 | 2.83×10^{-7} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 20 ⁰ 0 | 12051.57 | 1.44×10^{-11} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 10 ⁰ 0 | 12087.88 | 1.04×10^{-9} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 20 ⁰ 0 | 12089.73 | 1.26×10^{-9} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 00 ⁰ 1 | 12090.09 | 2.31×10^{-10} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 00 ⁰ 0 | 12123.85 | 7.52×10^{-8} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 10 ⁰ 0 | 12126.69 | 9.31×10^{-8} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 00 ⁰ 0 | 12162.97 | 6.87×10^{-6} |

TABLE 3. TRANSITIONS IN THE $J=2\leftarrow 1$ REGION OF OCS, ORDERED ACCORDING TO ABSORPTION COEFFICIENT IN NATURAL ABUNDANCE, AT 293K

| v_1 | v_2 | v_3 | ν/MHz | $\alpha_{\text{max}}/\text{cm}^{-1}$ | v_1 | v_2 | v_3 | ν/MHz | $\alpha_{\text{max}}/\text{cm}^{-1}$ | | |
|---|-------|----------------|------------------|--------------------------------------|-----------------------|---|-------|------------------|--------------------------------------|-----------------------|------------------------|
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 0 | 24325.92 | 5.38×10^{-5} | $^{18}\text{O}^{13}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 0 | 22764.240 | 9.89×10^{-10} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 0 | 24355.58 | 2.99×10^{-6} | $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 2 | 1 ¹ | 0 | 24219.54 | 5.51×10^{-10} |
| | | | | 24381.00 | 2.99×10^{-6} | | | | | 24248.68 | 5.51×10^{-10} |
| $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | 0 | 0 ⁰ | 0 | 23731.29 | 2.22×10^{-6} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 2 ⁰ | 0 | 22891.663 | 5.22×10^{-10} |
| | | | | | | $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 1 | 1 ¹ | 0 | 24208.276 | 4.90×10^{-10} |
| | | | | | | | | | | 24236.538 | 4.92×10^{-10} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 1 | 0 ⁰ | 0 | 24253.38 | 7.31×10^{-7} | $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | 2 | 0 ⁰ | 0 | 23588.44 | 4.59×10^{-10} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 0 | 24247.668 | 5.89×10^{-7} | $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 1 | 0 ⁰ | 0 | 23576.55 | 3.58×10^{-10} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 2 ⁰ | 0 | 24400.72 | 2.95×10^{-7} | $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 1 | 3 ¹ | 0 | 24348.2 | 2.36×10^{-10} |
| $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | 0 | 1 ¹ | 0 | 23760.48 | 1.24×10^{-7} | | | | | 24400.2 | 2.38×10^{-10} |
| | | | | 23784.74 | 1.24×10^{-7} | $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ | 0 | 1 ¹ | 0 | 22268.57 | 2.12×10^{-10} |
| | | | | | | | | | | 22290.14 | 2.13×10^{-10} |
| $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 0 | 22819.404 | 9.03×10^{-8} | $^{16}\text{O}^{13}\text{C}^{34}\text{S}$ | 0 | 2 ⁰ | 0 | 23715.43 ^a | 1.56×10^{-10} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 1 | 1 ¹ | 0 | 24288.36 | 4.18×10^{-8} | $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 2 | 0 ⁰ | 0 | 24102.54 | 1.14×10^{-10} |
| | | | | 24315.82 | 4.20×10^{-8} | $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 1 | 24212.10 ^a | 1.01×10^{-10} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 0 | 24274.60 | 3.53×10^{-8} | | | | | 24237.90 ^a | 1.01×10^{-10} |
| | | | | 24300.64 | 3.54×10^{-8} | | | | | | |
| $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | 1 | 0 ⁰ | 0 | 23660.56 | 3.19×10^{-8} | $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 5 ¹ | 0 | 24450.53 ^a | 8.81×10^{-11} |
| $^{16}\text{O}^{13}\text{C}^{34}\text{S}$ | 0 | 0 ⁰ | 0 | 23646.888 | 2.43×10^{-8} | | | | | 24523.19 ^a | 8.81×10^{-11} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 3 ¹ | 0 | 24409.74 | 1.64×10^{-8} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 1 | 1 ¹ | 0 | 22788.585 | 7.77×10^{-11} |
| | | | | 24459.20 | 1.64×10^{-8} | | | | | 22812.77 | 7.80×10^{-11} |
| $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | 0 | 2 ⁰ | 0 | 23804.97 | 1.22×10^{-8} | $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | 0 | 0 ⁰ | 1 | 23589.52 | 7.51×10^{-11} |
| | | | | | | $^{18}\text{O}^{13}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 0 | 22790.88 | 6.09×10^{-11} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 2 | 0 ⁰ | 0 | 24179.46 | 9.92×10^{-9} | | | | | 22814.034 | 6.11×10^{-11} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 1 | 0 ⁰ | 0 | 24175.751 | 8.18×10^{-9} | $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ | 1 | 0 ⁰ | 0 | 22176.76 | 5.93×10^{-11} |
| $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 0 | 22848.653 | 5.15×10^{-9} | $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 1 | 2 ⁰ | 0 | 24254.68 | 5.22×10^{-11} |
| | | | | 22871.228 | 5.16×10^{-9} | $^{18}\text{O}^{13}\text{C}^{34}\text{S}$ | 0 | 0 ⁰ | 0 | 22179.42 | 4.06×10^{-11} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 1 | 2 ⁰ | 0 | 24337.50 | 4.01×10^{-9} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 3 ¹ | 0 | 22902.513 | 2.96×10^{-11} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 0 | 2 ⁰ | 0 | 24316.962 | 3.76×10^{-9} | | | | | 22946.543 | 2.98×10^{-11} |
| $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ | 0 | 0 ⁰ | 0 | 22239.850 | 3.71×10^{-9} | $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 1 | 24110.60 | 2.61×10^{-11} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 1 | 24180.17 | 1.82×10^{-9} | $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 0 | 4 ⁰ | 0 | 24368.76 | 2.38×10^{-11} |
| $^{16}\text{O}^{13}\text{C}^{34}\text{S}$ | 0 | 1 ¹ | 0 | 23673.41 | 1.46×10^{-9} | $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ | 0 | 2 ⁰ | 0 | 22310.87 | 2.16×10^{-11} |
| | | | | 23698.20 | 1.46×10^{-9} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 2 | 0 ⁰ | 0 | 22688.524 | 2.05×10^{-11} |
| $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 1 | 0 ⁰ | 0 | 22754.570 | 1.36×10^{-9} | | | | | | |

^a Frequency estimated from the available rotational constants.

TABLE 4. TRANSITIONS IN THE $J=2+1$ REGION OF OCS, ORDERED ACCORDING TO FREQUENCY.
PEAK ABSORPTION COEFFICIENTS ARE CALCULATED FOR NATURAL ABUNDANCE AND 293 K

| $v_1 v_2^L v_3$ | ν/MHz | $\alpha_{\text{max}}/\text{cm}^{-1}$ | $v_1 v_2^L v_3$ | ν/MHz | $\alpha_{\text{max}}/\text{cm}^{-1}$ |
|--|----------------------|--------------------------------------|--|------------------------|--------------------------------------|
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 0 5 ¹ 0 | 24523.19 | 8.89×10^{-11} | $^{16}\text{O}^{12}\text{C}^{33}\text{S}$ 0 0 ⁰ 0 | 24019.641 ^b | |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 0 3 ¹ 0 | 24459.20 | 1.64×10^{-8} | $^{16}\text{O}^{12}\text{C}^{33}\text{S}$ 1 0 ⁰ 0 | 23947.4 ^b | |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 0 5 ¹ 0 | 24450.53 | 8.89×10^{-11} | $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ 0 2 ⁰ 0 | 23804.97 | 1.22×10^{-8} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 0 3 ¹ 0 | 24409.74 | 1.64×10^{-8} | $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ 0 1 ¹ 0 | 23784.74 | 1.24×10^{-7} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 0 2 ⁰ 0 | 24400.72 | 2.95×10^{-7} | $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ 0 1 ¹ 0 | 23760.48 | 1.24×10^{-7} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 1 3 ¹ 0 | 24400.2 | 2.38×10^{-10} | $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ 0 0 ⁰ 0 | 23731.29 | 2.22×10^{-6} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 0 1 ¹ 0 | 24381.00 | 2.99×10^{-6} | $^{16}\text{O}^{13}\text{C}^{34}\text{S}$ 0 2 ⁰ 0 | 23715.43 ^a | 1.56×10^{-10} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ 0 3 ¹ 0 | 24373.26 | 2.25×10^{-10} | $^{16}\text{O}^{13}\text{C}^{34}\text{S}$ 0 1 ¹ 0 | 23698.20 | 1.46×10^{-9} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ 0 4 ⁰ 0 | 24368.76 | 2.38×10^{-11} | $^{16}\text{O}^{13}\text{C}^{34}\text{S}$ 0 1 ¹ 0 | 23673.41 | 1.46×10^{-9} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 0 1 ¹ 0 | 24355.58 | 2.99×10^{-6} | $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ 1 0 ⁰ 0 | 23660.56 | 3.19×10^{-8} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 1 3 ¹ 0 | 24348.2 | 2.36×10^{-6} | $^{16}\text{O}^{13}\text{C}^{34}\text{S}$ 0 0 ⁰ 0 | 23646.888 | 2.43×10^{-8} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 1 2 ⁰ 0 | 24337.50 | 4.01×10^{-9} | $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ 0 0 ⁰ 1 | 23589.52 | 7.51×10^{-11} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 0 0 ⁰ 0 | 24325.92 | 5.38×10^{-5} | $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ 2 0 ⁰ 0 | 23588.44 | 4.59×10^{-10} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ 0 3 ¹ 0 | 24322.92 | 2.24×10^{-10} | $^{16}\text{O}^{13}\text{C}^{34}\text{S}$ 1 0 ⁰ 0 | 23576.55 | 3.58×10^{-10} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ 0 2 ⁰ 0 | 24316.962 | 3.76×10^{-9} | $^{17}\text{O}^{12}\text{C}^{32}\text{S}$ 0 0 ⁰ 0 | 23534.66 ^b | |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 1 1 ¹ 0 | 24315.82 | 4.20×10^{-8} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ 0 3 ¹ 0 | 22946.541 | 2.98×10^{-11} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ 0 1 ¹ 0 | 24300.64 | 3.54×10^{-8} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ 0 3 ¹ 0 | 22902.513 | 2.96×10^{-11} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 1 1 ¹ 0 | 24288.36 | 4.18×10^{-8} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ 0 2 ⁰ 0 | 22891.663 | 5.22×10^{-10} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ 0 1 ¹ 0 | 24274.60 | 3.53×10^{-8} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ 0 1 ¹ 0 | 22871.228 | 5.15×10^{-9} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ 1 2 ⁰ 0 | 24254.68 | 5.22×10^{-11} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ 0 1 ¹ 0 | 22848.653 | 5.15×10^{-9} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 1 0 ⁰ 0 | 24253.38 | 7.31×10^{-7} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ 1 2 ⁰ 0 | 22835.26 | 7.89×10^{-12} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 2 1 ¹ 0 | 24248.68 | 5.51×10^{-10} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ 0 0 ⁰ 0 | 22819.404 | 9.03×10^{-8} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ 0 0 ⁰ 0 | 24247.668 | 5.89×10^{-7} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ 0 1 ¹ 0 | 22814.034 | 6.11×10^{-11} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 0 1 ¹ 1 | 24237.90 | 1.01×10^{-10} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ 1 1 ¹ 0 | 22812.773 | 7.80×10^{-11} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ 1 1 ¹ 0 | 24236.538 | 4.92×10^{-10} | $^{18}\text{O}^{13}\text{C}^{32}\text{S}$ 0 1 ¹ 0 | 22790.88 | 6.09×10^{-11} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 2 1 ¹ 0 | 24219.54 | 5.51×10^{-10} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ 1 1 ¹ 0 | 22788.585 | 7.77×10^{-11} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 0 1 ¹ 1 | 24212.10 | 1.01×10^{-10} | $^{18}\text{O}^{13}\text{C}^{32}\text{S}$ 0 0 ⁰ 0 | 22764.240 | 9.89×10^{-10} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ 1 1 ¹ 0 | 24208.276 | 4.90×10^{-10} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ 1 0 ⁰ 0 | 22754.570 | 1.36×10^{-9} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 0 0 ⁰ 1 | 24180.17 | 1.82×10^{-9} | $^{18}\text{O}^{13}\text{C}^{32}\text{S}$ 1 0 ⁰ 0 | 22699.94 | 1.52×10^{-11} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ 2 0 ⁰ 0 | 24179.46 | 9.92×10^{-9} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ 2 0 ⁰ 0 | 22688.524 | 2.05×10^{-11} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ 1 0 ⁰ 0 | 24175.751 | 8.18×10^{-9} | $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ 0 2 ⁰ 0 | 22310.87 | 2.16×10^{-11} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ 0 0 ⁰ 1 | 24110.60 | 2.61×10^{-11} | $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ 0 1 ¹ 0 | 22290.14 | 2.13×10^{-10} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ 2 0 ⁰ 0 | 24102.54 | 1.14×10^{-10} | $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ 0 1 ¹ 0 | 22268.57 | 2.12×10^{-10} |
| $^{16}\text{O}^{12}\text{C}^{33}\text{S}$ 0 2 ⁰ 0 | 24092.4 ^b | | $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ 0 0 ⁰ 0 | 22239.850 | 3.71×10^{-9} |
| $^{16}\text{O}^{12}\text{C}^{33}\text{S}$ 0 1 ¹ 0 | 24074.2 ^b | | $^{18}\text{O}^{13}\text{C}^{34}\text{S}$ 0 0 ⁰ 0 | 22179.42 | 4.06×10^{-11} |
| $^{16}\text{O}^{12}\text{C}^{33}\text{S}$ 0 1 ¹ 0 | 24049.4 ^b | | $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ 1 0 ⁰ 0 | 22176.76 | 5.93×10^{-11} |

^aFrequency estimated from the available rotational constants.

^bCalculated nuclear quadrupole unsplit frequency.

TABLE 5. TRANSITIONS IN THE $J=3+2$ REGION OF OCS, ORDERED ACCORDING TO THE PEAK ABSORPTION COEFFICIENT IN NATURAL ABUNDANCE, AT 293 K

| v_1 | v_2 | v_3 | ν/MHz | $\alpha_{\text{max}}/\text{cm}^{-1}$ | v_1 | v_2 | v_3 | ν/MHz | $\alpha_{\text{max}}/\text{cm}^{-1}$ | | |
|---|-------|----------------|------------------|--------------------------------------|-----------------------|---|-------|-----------------------|--------------------------------------|------------------------|------------------------|
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 0 | 36488.8128 | 1.78×10^{-4} | $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 2 | 1 ¹ | 0 | 36372.95 ^b | 2.17×10^{-9} |
| | | | | | | | | 36329.24 ^b | 2.16×10^{-9} | | |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 0 | 36533.26 ^a | 1.17×10^{-5} | $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 1 | 1 ¹ | 0 | 36312.34 ^b | 1.92×10^{-9} |
| | | | | 36571.41 ^a | 1.17×10^{-5} | | | 36354.73 ^b | 1.93×10^{-9} | | |
| $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | 0 | 0 ⁰ | 0 | 35596.91 | 7.32×10^{-6} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 2 ² | 0 | 34350.073 ^c | 1.92×10^{-9} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 1 | 0 ⁰ | 0 | 36380.00 ^b | 2.42×10^{-6} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 2 ⁰ | 0 | 34337.45 | 1.73×10^{-9} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 0 | 36371.390 | 1.95×10^{-6} | $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | 2 | 0 ⁰ | 0 | 35382.60 ^b | 1.52×10^{-9} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 2 ² | 0 | 36615.26 ^{a,c} | 1.08×10^{-6} | $^{16}\text{O}^{13}\text{C}^{34}\text{S}$ | 1 | 0 ⁰ | 0 | 35364.78 ^b | 1.18×10^{-9} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 2 ⁰ | 0 | 36601.03 ^a | 9.74×10^{-7} | $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 1 | 3 ¹ | 0 | 36522.24 ^b | 9.25×10^{-10} |
| $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | 0 | 1 ¹ | 0 | 35640.66 | 4.84×10^{-7} | | | 36600.24 ^b | 9.31×10^{-10} | | |
| | | | | 35676.98 | 4.85×10^{-7} | $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 0 | 3 ¹ | 0 | 36484.348 | 8.76×10^{-10} |
| $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 0 | 34229.045 | 2.98×10^{-7} | | | 36559.81 | 8.82×10^{-10} | | |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 1 | 1 ¹ | 0 | 36432.29 | 1.64×10^{-7} | $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ | 0 | 1 ¹ | 0 | 33402.80 ^b | 8.31×10^{-10} |
| | | | | 36473.47 | 1.64×10^{-7} | | | 33435.15 ^b | 8.34×10^{-10} | | |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 0 | 36411.84 ^b | 1.38×10^{-7} | $^{16}\text{O}^{13}\text{C}^{34}\text{S}$ | 0 | 2 ² | 0 | 35586.22 ^c | 5.74×10^{-10} |
| | | | | 36450.876 | 1.39×10^{-7} | $^{16}\text{O}^{13}\text{C}^{34}\text{S}$ | 0 | 2 ⁰ | 0 | 35573.06 | 5.16×10^{-10} |
| $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | 1 | 0 ⁰ | 0 | 35490.77 | 1.05×10^{-7} | $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 1 | 36318.08 | 3.95×10^{-10} |
| | | | | | | | | 36356.78 | 3.96×10^{-10} | | |
| $^{16}\text{O}^{13}\text{C}^{34}\text{S}$ | 0 | 0 ⁰ | 0 | 35470.264 | 8.02×10^{-8} | $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 2 | 0 ⁰ | 0 | 36153.67 | 3.75×10^{-10} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 3 ¹ | 0 | 36614.53 ^b | 6.37×10^{-8} | $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 5 ¹ | 0 | 36675.75 | 3.45×10^{-10} |
| | | | | 36688.73 ^b | 6.41×10^{-8} | | | 36784.74 | 3.48×10^{-10} | | |
| $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | 0 | 2 ² | 0 | 35720.27 ^c | 4.50×10^{-8} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 1 | 1 ¹ | 0 | 34182.85 | 3.04×10^{-10} |
| $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | 0 | 2 ⁰ | 0 | 35707.50 | 4.05×10^{-8} | | | 34219.151 | 3.05×10^{-10} | | |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 2 | 0 ⁰ | 0 | 36269.10 ^b | 3.28×10^{-8} | $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | 0 | 0 ⁰ | 1 | 35384.22 ^b | 2.48×10^{-10} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 1 | 0 ⁰ | 0 | 36263.46 | 2.70×10^{-8} | $^{18}\text{O}^{13}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 0 | 34186.27 ^b | 2.39×10^{-10} |
| $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 0 | 34272.920 | 2.02×10^{-8} | | | 34221.116 | 2.39×10^{-10} | | |
| | | | | 34306.73 | 2.02×10^{-8} | $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ | 1 | 0 ⁰ | 0 | 33265.09 ^b | 1.96×10^{-10} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 1 | 2 ² | 0 | 36523.38 ^c | 1.47×10^{-8} | $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 1 | 2 ² | 0 | 36400.79 ^c | 1.92×10^{-10} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 0 | 2 ² | 0 | 36490.723 ^c | 1.38×10^{-8} | $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 1 | 2 ⁰ | 0 | 36381.96 ^b | 1.73×10^{-10} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 1 | 2 ⁰ | 0 | 36506.19 ^b | 1.33×10^{-8} | $^{18}\text{O}^{13}\text{C}^{34}\text{S}$ | 0 | 0 ⁰ | 0 | 33269.1 | 1.34×10^{-10} |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 0 | 2 ⁰ | 0 | 36475.38 | 1.24×10^{-8} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 3 ¹ | 0 | 34353.748 | 1.16×10^{-10} |
| $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ | 0 | 0 ⁰ | 0 | 33359.71 ^b | 1.23×10^{-8} | | | 34419.83 | 1.17×10^{-10} | | |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 1 | 36270.17 ^b | 6.01×10^{-9} | $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 0 | 4 ² | 0 | 36607.49 ^c | 8.78×10^{-11} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 0 | 4 ² | 0 | 36703.77 ^c | 5.90×10^{-9} | $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 1 | 36165.72 | 8.61×10^{-11} |
| $^{16}\text{O}^{13}\text{C}^{34}\text{S}$ | 0 | 1 ¹ | 0 | 35510.08 ^b | 5.72×10^{-9} | $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 0 | 4 ⁰ | 0 | 36553.08 ^b | 7.86×10^{-11} |
| | | | | 35547.27 ^b | 5.73×10^{-9} | $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ | 0 | 2 ⁰ | 0 | 33466.25 ^b | 7.14×10^{-11} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 1 | 0 ⁰ | 0 | 34131.83 | 4.50×10^{-9} | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 2 | 0 ⁰ | 0 | 34032.79 ^b | 6.79×10^{-11} |
| $^{18}\text{O}^{13}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 0 | 34146.30 ^b | 3.27×10^{-9} | $^{18}\text{O}^{13}\text{C}^{32}\text{S}$ | 1 | 0 ⁰ | 0 | 34049.86 ^b | 5.02×10^{-11} |
| | | | | | | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 1 | 2 ² | 0 | 34268.13 | 2.90×10^{-11} |
| | | | | | | $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 1 | 2 ⁰ | 0 | 34252.84 | 2.61×10^{-11} |

^aFrequency remeasured in this work.

^bFrequency estimated from the available rotational constants.

^cUnresolved doublet.

TABLE 6. TRANSITIONS IN THE $J=3\leftarrow 2$ REGION OF OCS, ORDERED ACCORDING TO FREQUENCY,

PEAK ABSORPTION COEFFICIENTS ARE CALCULATED FOR NATURAL ABUNDANCE AND 293K

| v_1 | v_2 | v_3 | ν/MHz | $\alpha_{\text{max}}/\text{cm}^{-1}$ | v_1 | v_2 | v_3 | ν/MHz | $\alpha_{\text{max}}/\text{cm}^{-1}$ | | |
|-------------------------------------|-------|----------------|------------------|--------------------------------------|------------------------|-------------------------------------|-------|------------------|--------------------------------------|-------------------------|------------------------|
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 0 | 5 ¹ | 0 | 36784.74 | 3.84×10^{-10} | $^{16}_0^{12}\text{C}^{33}\text{S}$ | 0 | 1 ¹ | 0 | 36074.07 ^{b,c} | |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 0 | 4 ² | 0 | 36703.77 ^d | 5.90×10^{-9} | $^{16}_0^{12}\text{C}^{33}\text{S}$ | 0 | 0 ⁰ | 0 | 36029.39 ^{b,c} | |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 0 | 3 ¹ | 0 | 36688.73 ^b | 9.74×10^{-8} | $^{16}_0^{12}\text{C}^{33}\text{S}$ | 1 | 0 ⁰ | 0 | 35921.02 ^{b,c} | |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 0 | 5 ¹ | 0 | 36675.75 | 3.45×10^{-10} | $^{16}_0^{12}\text{C}^{34}\text{S}$ | 0 | 2 ² | 0 | 35720.27 ^d | 4.50×10^{-8} |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 0 | 2 ² | 0 | 36615.26 ^{a,d} | 1.08×10^{-6} | $^{16}_0^{12}\text{C}^{34}\text{S}$ | 0 | 2 ⁰ | 0 | 35707.50 | 4.05×10^{-8} |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 0 | 3 ¹ | 0 | 36614.53 ^b | 6.37×10^{-8} | $^{16}_0^{12}\text{C}^{34}\text{S}$ | 0 | 1 ¹ | 0 | 35676.98 | 4.85×10^{-7} |
| $^{16}_0^{13}\text{C}^{32}\text{S}$ | 0 | 4 ² | 0 | 36607.49 ^d | 8.78×10^{-11} | $^{16}_0^{12}\text{C}^{34}\text{S}$ | 0 | 1 ¹ | 0 | 35640.66 | 4.84×10^{-7} |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 0 | 2 ⁰ | 0 | 36601.03 ^a | 9.74×10^{-7} | $^{16}_0^{12}\text{C}^{34}\text{S}$ | 0 | 0 ⁰ | 0 | 35596.91 | 7.32×10^{-6} |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 1 | 3 ¹ | 0 | 36600.24 ^b | 9.31×10^{-10} | $^{16}_0^{13}\text{C}^{34}\text{S}$ | 0 | 2 ² | 0 | 35586.22 ^d | 5.74×10^{-10} |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 0 | 36571.41 ^a | 1.17×10^{-7} | $^{16}_0^{13}\text{C}^{34}\text{S}$ | 0 | 2 ⁰ | 0 | 35573.06 | 5.16×10^{-10} |
| $^{16}_0^{13}\text{C}^{32}\text{S}$ | 0 | 3 ¹ | 0 | 36559.81 | 8.82×10^{-10} | $^{16}_0^{13}\text{C}^{34}\text{S}$ | 0 | 1 ¹ | 0 | 35547.27 ^b | 5.73×10^{-9} |
| $^{16}_0^{13}\text{C}^{32}\text{S}$ | 0 | 4 ⁰ | 0 | 36553.08 ^b | 7.86×10^{-11} | $^{16}_0^{13}\text{C}^{34}\text{S}$ | 0 | 1 ¹ | 0 | 35510.08 ^b | 5.72×10^{-9} |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 0 | 36533.26 ^a | 1.17×10^{-5} | $^{16}_0^{12}\text{C}^{34}\text{S}$ | 1 | 0 ⁰ | 0 | 35490.77 | 1.05×10^{-7} |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 1 | 2 ² | 0 | 36523.38 ^d | 1.47×10^{-8} | $^{16}_0^{13}\text{C}^{34}\text{S}$ | 0 | 0 ⁰ | 0 | 35470.264 | 8.02×10^{-8} |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 1 | 3 ¹ | 0 | 36522.24 ^b | 9.25×10^{-10} | $^{16}_0^{12}\text{C}^{34}\text{S}$ | 0 | 0 ⁰ | 1 | 35384.22 ^b | 4.84×10^{-10} |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 1 | 2 ⁰ | 0 | 36506.19 ^b | 1.33×10^{-8} | $^{16}_0^{12}\text{C}^{34}\text{S}$ | 2 | 0 ⁰ | 0 | 35382.60 ^b | 1.52×10^{-9} |
| $^{16}_0^{13}\text{C}^{32}\text{S}$ | 0 | 2 ² | 0 | 36490.723 ^d | 1.38×10^{-8} | $^{16}_0^{13}\text{C}^{34}\text{S}$ | 1 | 0 ⁰ | 0 | 35364.78 ^b | 1.18×10^{-9} |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 0 | 36488.8128 | 1.78×10^{-4} | $^{18}_0^{12}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 0 | 35301.92 ^{b,c} | |
| $^{16}_0^{13}\text{C}^{32}\text{S}$ | 0 | 3 ¹ | 0 | 36484.348 | 8.76×10^{-10} | $^{18}_0^{12}\text{C}^{32}\text{S}$ | 0 | 3 ¹ | 0 | 34419.83 | 1.17×10^{-10} |
| $^{16}_0^{13}\text{C}^{32}\text{S}$ | 0 | 2 ⁰ | 0 | 36475.38 | 1.24×10^{-8} | $^{18}_0^{12}\text{C}^{32}\text{S}$ | 0 | 3 ¹ | 0 | 34353.748 | 1.16×10^{-10} |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 1 | 1 ¹ | 0 | 36473.47 | 1.64×10^{-7} | $^{18}_0^{12}\text{C}^{32}\text{S}$ | 0 | 2 ² | 0 | 34350.073 ^d | 1.92×10^{-10} |
| $^{16}_0^{13}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 0 | 36450.876 | 1.39×10^{-7} | $^{18}_0^{12}\text{C}^{32}\text{S}$ | 0 | 2 ⁰ | 0 | 34337.45 | 1.73×10^{-9} |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 1 | 1 ¹ | 0 | 36432.29 | 1.64×10^{-7} | $^{18}_0^{12}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 0 | 34306.73 | 2.02×10^{-8} |
| $^{16}_0^{13}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 0 | 36411.84 ^b | 1.38×10^{-7} | $^{18}_0^{12}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 0 | 34272.920 | 2.02×10^{-8} |
| $^{16}_0^{13}\text{C}^{32}\text{S}$ | 1 | 2 ² | 0 | 36400.79 ^d | 1.92×10^{-10} | $^{18}_0^{12}\text{C}^{32}\text{S}$ | 1 | 2 ⁰ | 0 | 34252.84 | 2.61×10^{-11} |
| $^{16}_0^{13}\text{C}^{32}\text{S}$ | 1 | 2 ⁰ | 0 | 36381.96 ^b | 1.73×10^{-10} | $^{18}_0^{12}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 0 | 34229.045 | 2.98×10^{-7} |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 1 | 0 ⁰ | 0 | 36380.00 ^b | 2.42×10^{-6} | $^{18}_0^{13}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 0 | 34221.116 | 2.39×10^{-10} |
| $^{16}_0^{13}\text{C}^{32}\text{S}$ | 2 | 1 ¹ | 0 | 36372.95 ^b | 2.17×10^{-9} | $^{18}_0^{12}\text{C}^{32}\text{S}$ | 1 | 1 ¹ | 0 | 34219.151 | 3.05×10^{-10} |
| $^{16}_0^{13}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 0 | 36371.390 | 1.95×10^{-6} | $^{18}_0^{13}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 0 | 34186.27 ^b | 2.39×10^{-10} |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 1 | 36356.78 | 3.96×10^{-10} | $^{18}_0^{12}\text{C}^{32}\text{S}$ | 1 | 1 ¹ | 0 | 34182.85 | 3.04×10^{-10} |
| $^{16}_0^{13}\text{C}^{32}\text{S}$ | 1 | 1 ¹ | 0 | 36354.73 ^b | 1.93×10^{-9} | $^{18}_0^{13}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 0 | 34146.30 ^b | 3.27×10^{-9} |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 2 | 1 ¹ | 0 | 36329.24 ^b | 2.16×10^{-9} | $^{18}_0^{12}\text{C}^{32}\text{S}$ | 1 | 0 ⁰ | 0 | 34131.83 | 4.50×10^{-9} |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 0 | 1 ¹ | 1 | 36318.08 | 3.95×10^{-10} | $^{18}_0^{13}\text{C}^{32}\text{S}$ | 1 | 0 ⁰ | 0 | 34049.86 ^b | 5.02×10^{-11} |
| $^{16}_0^{13}\text{C}^{32}\text{S}$ | 1 | 1 ¹ | 0 | 36312.34 ^b | 1.92×10^{-9} | $^{18}_0^{12}\text{C}^{32}\text{S}$ | 2 | 0 ⁰ | 0 | 34032.79 ^b | 6.79×10^{-11} |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 1 | 36270.17 ^b | 6.01×10^{-9} | $^{18}_0^{12}\text{C}^{34}\text{S}$ | 0 | 2 ⁰ | 0 | 33466.25 ^b | 7.14×10^{-11} |
| $^{16}_0^{12}\text{C}^{32}\text{S}$ | 2 | 0 ⁰ | 0 | 36269.10 ^b | 3.78×10^{-8} | $^{18}_0^{12}\text{C}^{34}\text{S}$ | 0 | 1 ¹ | 0 | 33435.15 ^b | 8.34×10^{-10} |
| $^{16}_0^{13}\text{C}^{32}\text{S}$ | 1 | 0 ⁰ | 0 | 36263.46 | 2.70×10^{-8} | $^{18}_0^{12}\text{C}^{34}\text{S}$ | 0 | 1 ¹ | 0 | 33402.80 ^b | 8.31×10^{-10} |
| $^{16}_0^{13}\text{C}^{32}\text{S}$ | 0 | 0 ⁰ | 1 | 36165.72 | 8.61×10^{-11} | $^{18}_0^{12}\text{C}^{34}\text{S}$ | 0 | 0 ⁰ | 0 | 33359.71 ^b | 1.23×10^{-8} |
| $^{16}_0^{13}\text{C}^{32}\text{S}$ | 2 | 0 ⁰ | 0 | 36153.67 | 3.75×10^{-10} | $^{18}_0^{13}\text{C}^{34}\text{S}$ | 0 | 0 ⁰ | 0 | 33269.1 | 1.34×10^{-10} |
| $^{16}_0^{12}\text{C}^{33}\text{S}$ | 0 | 2 ⁰ | 0 | 36138.52 ^{b,c} | | $^{18}_0^{12}\text{C}^{34}\text{S}$ | 1 | 0 ⁰ | 0 | 33265.09 ^b | 1.96×10^{-10} |
| $^{16}_0^{12}\text{C}^{33}\text{S}$ | 0 | 1 ¹ | 0 | 36111.33 ^{b,c} | | | | | | | |

^aFrequency remeasured in this work.^bFrequency estimated from the available rotational constants.^cCalculated nuclear quadrupole unsplit frequency.^dUnresolved doublet.

TABLE 7. Transitions in regions $J = J' + J''$, each ordered according to frequency, for $J' = 4$ to 25 and $J'' = 3$ to 24

| J = 4 ← 3 | | | | J = 5 ← 4 | | | |
|-------------------|-------------|----------------|-----------------|-------------------|-------------|----------------|-----------------|
| ISOTOPIIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 | ISOTOPIIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 |
| 0.16 C.12 S.32 | 0 0.0 0 | 48651.61 | 4.14E-04 | 0.16 C.12 S.32 | 0 0.0 0 | 60814.27 | 7.89E-04 |
| | 0 1.1 0 | 48710.86 | 2.87E-05 | | 0 1.1 0 | 60888.34 | 5.61E-05 |
| | 0 1.1 0 | 48761.75 | 2.87E-05 | | 0 1.1 0 | 60951.95 | 5.61E-05 |
| 0.16 C.12 S.34 | 0 0.0 0 | 47462.36 | 1.70E-05 | 0.16 C.12 S.34 | 0 0.0 0 | 59327.73 | 3.25E-05 |
| | 0 1.1 0 | 47520.8 | 1.19E-06 | | 0 1.1 0 | 59400.8 | 2.32E-06 |
| | 0 1.1 0 | 47569.4 | 1.19E-06 | | 0 1.1 0 | 59461.5 | 2.32E-06 |
| 0.16 C.13 S.32 | 0 0.0 0 | 48495.07 | 4.53E-06 | 0.16 C.13 S.32 | 0 0.0 0 | 60618.60 | 8.64E-06 |
| | 0 1.1 0 | 48549.0 | 3.39E-07 | | 0 1.1 0 | 60686.0 | 6.62E-07 |
| | 0 1.1 0 | 48601.0 | 3.39E-07 | | 0 1.1 0 | 60751.1 | 6.62E-07 |
| 0.18 C.12 S.32 | 0 0.0 0 | 45638.59 | 6.95E-07 | 0.18 C.12 S.32 | 0 0.0 0 | 57048.04 | 1.33E-06 |
| | 0 1.1 0 | 45697.1 | 4.95E-08 | | 0 1.1 0 | 57121.1 | 9.68E-08 |
| | 0 1.1 0 | 45742.3 | 4.95E-08 | | 0 1.1 0 | 57177.6 | 9.68E-08 |
| 0.16 C.13 S.34 | 0 0.0 0 | 47293.5 | 1.87E-07 | 0.16 C.13 S.34 | 0 0.0 0 | 59116.7 | 3.56E-07 |
| | 0 1.1 0 | 47346.6 | 1.40E-08 | | 0 1.1 0 | 59183.0 | 2.74E-08 |
| | 0 1.1 0 | 47396.2 | 1.40E-08 | | 0 1.1 0 | 59245.0 | 2.74E-08 |
| 0.18 C.12 S.34 | 0 0.0 0 | 44479.5 | 2.85E-08 | 0.18 C.12 S.34 | 0 0.0 0 | 55599.2 | 5.45E-08 |
| | 0 1.1 0 | 44537.2 | 2.04E-09 | | 0 1.1 0 | 55671.4 | 3.99E-09 |
| | 0 1.1 0 | 44580.1 | 2.04E-09 | | 0 1.1 0 | 55724.9 | 3.99E-09 |
| 0.18 C.13 S.32 | 0 0.0 0 | 45528.3 | 7.61E-09 | 0.18 C.13 S.32 | 0 0.0 0 | 56910.1 | 1.45E-08 |
| | 0 1.1 0 | 45581.5 | 5.86E-10 | | 0 1.1 0 | 56976.7 | 1.15E-09 |
| | 0 1.1 0 | 45627.9 | 5.86E-10 | | 0 1.1 0 | 57034.7 | 1.15E-09 |
| 0.18 C.13 S.34 | 0 0.0 0 | 44358.6 | 3.12E-10 | 0.18 C.13 S.34 | 0 0.0 0 | 55448.1 | 5.97E-10 |

| J = 6 ← 5 | | | | J = 7 ← 6 | | | |
|-------------------|-------------|----------------|-----------------|-------------------|-------------|----------------|-----------------|
| ISOTOPIIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 | ISOTOPIIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 |
| 0.16 C.12 S.32 | 0 0.0 0 | 72976.78 | 1.33E-03 | 0.16 C.12 S.32 | 0 0.0 0 | 85139.11 | 2.05E-03 |
| | 0 1.1 0 | 73065.66 | 9.55E-05 | | 0 1.1 0 | 85242.79 | 1.48E-04 |
| | 0 1.1 0 | 73141.99 | 9.55E-05 | | 0 1.1 0 | 85331.84 | 1.48E-04 |
| 0.16 C.12 S.34 | 0 0.0 0 | 71192.94 | 5.47E-05 | 0.16 C.12 S.34 | 0 0.0 0 | 83057.98 | 8.43E-05 |
| | 0 1.1 0 | 71280.6 | 3.95E-06 | | 0 1.1 0 | 83160.3 | 6.14E-06 |
| | 0 1.1 0 | 71353.5 | 3.95E-06 | | 0 1.1 0 | 83245.2 | 6.14E-06 |
| 0.16 C.13 S.32 | 0 0.0 0 | 72741.98 | 1.45E-05 | 0.16 C.13 S.32 | 0 0.0 0 | 84865.17 | 2.24E-05 |
| | 0 1.1 0 | 72822.8 | 1.13E-06 | | 0 1.1 0 | 84959.5 | 1.75E-06 |
| | 0 1.1 0 | 72900.9 | 1.13E-06 | | 0 1.1 0 | 85050.6 | 1.75E-06 |
| 0.18 C.12 S.32 | 0 0.0 0 | 68457.35 | 2.23E-06 | 0.18 C.12 S.32 | 0 0.0 0 | 79866.49 | 3.44E-06 |
| | 0 1.1 0 | 68545.0 | 1.65E-07 | | 0 1.1 0 | 79968.7 | 2.56E-07 |
| | 0 1.1 0 | 68612.9 | 1.65E-07 | | 0 1.1 0 | 80047.9 | 2.56E-07 |
| 0.16 C.13 S.34 | 0 0.0 0 | 70939.7 | 5.99E-07 | 0.16 C.13 S.34 | 0 0.0 0 | 82762.6 | 9.24E-07 |
| | 0 1.1 0 | 71019.3 | 4.67E-08 | | 0 1.1 0 | 82855.3 | 7.26E-08 |
| | 0 1.1 0 | 71093.6 | 4.67E-08 | | 0 1.1 0 | 82942.1 | 7.26E-08 |
| 0.18 C.12 S.34 | 0 0.0 0 | 66718.7 | 9.16E-08 | 0.18 C.12 S.34 | 0 0.0 0 | 77838.1 | 1.41E-07 |
| | 0 1.1 0 | 66805.7 | 6.80E-09 | | 0 1.1 0 | 77939.9 | 1.06E-08 |
| | 0 1.1 0 | 66869.5 | 6.80E-09 | | 0 1.1 0 | 78014.1 | 1.06E-08 |
| 0.18 C.13 S.32 | 0 0.0 0 | 68291.8 | 2.44E-08 | 0.18 C.13 S.32 | 0 0.0 0 | 79673.4 | 3.77E-08 |
| | 0 1.1 0 | 68371.7 | 1.95E-09 | | 0 1.1 0 | 79766.6 | 3.04E-09 |
| | 0 1.1 0 | 68441.3 | 1.95E-09 | | 0 1.1 0 | 79847.8 | 3.03E-09 |
| 0.18 C.13 S.34 | 0 0.0 0 | 66537.4 | 1.00E-09 | 0.18 C.13 S.34 | 0 0.0 0 | 77626.6 | 1.55E-09 |

TABLE 7. Transitions in regions $J = J' + J''$, each ordered according to frequency, for $J' = 4$ to 25 and $J'' = 3$ to 24--Continued

J = 8 ← 7

| ISOTOPIIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 |
|-------------------|-------------|----------------|-----------------|
| 0.16 C.12 S.32 | 0 0 0 0 | 97301.21 | 2.95E-03 |
| | 0 1 1 0 | 97419.69 | 2.15E-04 |
| | 0 1 1 0 | 97521.47 | 2.15E-04 |
| 0.16 C.12 S.34 | 0 0 0 0 | 94922.81 | 1.22E-04 |
| | 0 1 1 0 | 95039.7 | 8.91E-06 |
| | 0 1 1 0 | 95136.8 | 8.91E-06 |
| 0.16 C.13 S.32 | 0 0 0 0 | 96988.14 | 3.23E-05 |
| | 0 1 1 0 | 97095.9 | 2.54E-06 |
| | 0 1 1 0 | 97200.0 | 2.54E-06 |
| 0.18 C.12 S.32 | 0 0 0 0 | 91275.45 | 4.97E-06 |
| | 0 1 1 0 | 91392.3 | 3.72E-07 |
| | 0 1 1 0 | 91482.7 | 3.72E-07 |
| 0.16 C.13 S.34 | 0 0 0 0 | 94585.2 | 1.33E-06 |
| | 0 1 1 0 | 94691.2 | 1.05E-07 |
| | 0 1 1 0 | 94790.4 | 1.05E-07 |
| 0.18 C.12 S.34 | 0 0 0 0 | 88957.3 | 2.04E-07 |
| | 0 1 1 0 | 89074.1 | 1.54E-08 |
| | 0 1 1 0 | 89158.4 | 1.54E-08 |
| 0.18 C.13 S.32 | 0 0 0 0 | 91054.8 | 5.45E-08 |
| | 0 1 1 0 | 91161.2 | 4.41E-09 |
| | 0 1 1 0 | 91254.0 | 4.41E-09 |
| 0.18 C.13 S.34 | 0 0 0 0 | 88715.6 | 2.24E-09 |

J = 9 ← 8

| ISOTOPIIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 |
|-------------------|-------------|----------------|-----------------|
| 0.16 C.12 S.32 | 0 0 0 0 | 109463.07 | 4.06E-03 |
| | 0 1 1 0 | 109596.35 | 2.97E-04 |
| | 0 1 1 0 | 109710.85 | 2.97E-04 |
| 0.16 C.12 S.34 | 0 0 0 0 | 106787.40 | 1.67E-04 |
| | 0 1 1 0 | 106918.9 | 1.23E-05 |
| | 0 1 1 0 | 107028.2 | 1.23E-05 |
| 0.16 C.13 S.32 | 0 0 0 0 | 109110.86 | 4.44E-05 |
| | 0 1 1 0 | 109232.1 | 3.50E-06 |
| | 0 1 1 0 | 109349.2 | 3.50E-06 |
| 0.18 C.12 S.32 | 0 0 0 0 | 102684.18 | 6.84E-06 |
| | 0 1 1 0 | 102815.6 | 5.14E-07 |
| | 0 1 1 0 | 102917.3 | 5.14E-07 |
| 0.16 C.13 S.34 | 0 0 0 0 | 106407.6 | 1.84E-06 |
| | 0 1 1 0 | 106526.8 | 1.45E-07 |
| | 0 1 1 0 | 106638.4 | 1.45E-07 |
| 0.18 C.12 S.34 | 0 0 0 0 | 100076.3 | 2.81E-07 |
| | 0 1 1 0 | 100208.3 | 2.12E-08 |
| | 0 1 1 0 | 100302.5 | 2.12E-08 |
| 0.18 C.13 S.32 | 0 0 0 0 | 102435.9 | 7.50E-08 |
| | 0 1 1 0 | 102555.6 | 6.09E-09 |
| | 0 1 1 0 | 102660.0 | 6.08E-09 |
| 0.18 C.13 S.34 | 0 0 0 0 | 99804.4 | 3.08E-09 |

J = 10 ← 9

| ISOTOPIIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 |
|-------------------|-------------|----------------|-----------------|
| 0.16 C.12 S.32 | 0 0 0 0 | 121624.64 | 5.37E-03 |
| | 0 1 1 0 | 121772.71 | 3.93E-04 |
| | 0 1 1 0 | 121899.93 | 3.93E-04 |
| 0.16 C.12 S.34 | 0 0 0 0 | 118651.72 | 2.22E-04 |
| | 0 1 1 0 | 118798. | 1.63E-05 |
| | 0 1 1 0 | 118919. | 1.63E-05 |
| 0.16 C.13 S.32 | 0 0 0 0 | 121233.31 | 5.87E-05 |
| | 0 1 1 0 | 121368. | 4.64E-06 |
| | 0 1 1 0 | 121498. | 4.64E-06 |
| 0.18 C.12 S.32 | 0 0 0 0 | 114092.67 | 9.06E-06 |
| | 0 1 1 0 | 114239. | 6.82E-07 |
| | 0 1 1 0 | 114352. | 6.82E-07 |
| 0.16 C.13 S.34 | 0 0 0 0 | 118230. | 2.43E-06 |
| | 0 1 1 0 | 118362. | 1.93E-07 |
| | 0 1 1 0 | 118486. | 1.93E-07 |
| 0.18 C.12 S.34 | 0 0 0 0 | 111195. | 3.73E-07 |
| | 0 1 1 0 | 111342. | 2.82E-08 |
| | 0 1 1 0 | 111446. | 2.82E-08 |
| 0.18 C.13 S.32 | 0 0 0 0 | 113817. | 9.93E-08 |
| | 0 1 1 0 | 113950. | 8.07E-09 |
| | 0 1 1 0 | 114066. | 8.07E-09 |
| 0.18 C.13 S.34 | 0 0 0 0 | 110893. | 4.08E-09 |

J = 11 ← 10

| ISOTOPIIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 |
|-------------------|-------------|----------------|-----------------|
| 0.16 C.12 S.32 | 0 0 0 0 | 133785.90 | 6.87E-03 |
| | 0 1 1 0 | 133948.76 | 5.05E-04 |
| | 0 1 1 0 | 134088.70 | 5.05E-04 |
| 0.16 C.12 S.34 | 0 0 0 0 | 130515.74 | 2.84E-04 |
| | 0 1 1 0 | 130676. | 2.09E-05 |
| | 0 1 1 0 | 130810. | 2.09E-05 |
| 0.16 C.13 S.32 | 0 0 0 0 | 133355.44 | 7.52E-05 |
| | 0 1 1 0 | 133504. | 5.96E-06 |
| | 0 1 1 0 | 133647. | 5.96E-06 |
| 0.18 C.12 S.32 | 0 0 0 0 | 125500.89 | 1.16E-05 |
| | 0 1 1 0 | 125661. | 8.76E-07 |
| | 0 1 1 0 | 125786. | 8.76E-07 |
| 0.16 C.13 S.34 | 0 0 0 0 | 130052. | 3.11E-06 |
| | 0 1 1 0 | 130197. | 2.47E-07 |
| | 0 1 1 0 | 130334. | 2.47E-07 |
| 0.18 C.12 S.34 | 0 0 0 0 | 122314. | 4.78E-07 |
| | 0 1 1 0 | 122477. | 3.62E-08 |
| | 0 1 1 0 | 122590. | 3.62E-08 |
| 0.18 C.13 S.32 | 0 0 0 0 | 125197. | 1.27E-07 |
| | 0 1 1 0 | 125344. | 1.04E-08 |
| | 0 1 1 0 | 125471. | 1.04E-08 |
| 0.18 C.13 S.34 | 0 0 0 0 | 121981. | 5.24E-09 |

TABLE 7. Transitions in regions $J = J' + J''$, each ordered according to frequency, for $J' = 4$ to 25 and $J'' = 3$ to 24 --Continued

| J = 12 (- 11) | | | | J = 13 (- 12) | | | |
|------------------|-------------|----------------|-----------------|------------------|-------------|----------------|-----------------|
| ISOTOPIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 | ISOTOPIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 |
| 0.16 C.12 S.32 | 0 0.0 0 | 145946.82 | 8.57E-03 | 0.16 C.12 S.32 | 0 0.0 0 | 158107.36 | 1.05E-02 |
| | 0 1.1 0 | 146124.46 | 6.30E-04 | | 0 1.1 0 | 158299.78 | 7.69E-04 |
| | 0 1.1 0 | 146277.12 | 6.30E-04 | | 0 1.1 0 | 158465.16 | 7.69E-04 |
| 0.16 C.12 S.34 | 0 0.0 0 | 142379.44 | 3.54E-04 | 0.16 C.12 S.34 | 0 0.0 0 | 154242.77 | 4.32E-04 |
| | 0 1.1 0 | 142555. | 2.61E-05 | | 0 1.1 0 | 154433. | 3.19E-05 |
| | 0 1.1 0 | 142700. | 2.61E-05 | | 0 1.1 0 | 154590. | 3.19E-05 |
| 0.16 C.13 S.32 | 0 0.0 0 | 145477.22 | 9.38E-05 | 0.16 C.13 S.32 | 0 0.0 0 | 157598.64 | 1.14E-04 |
| | 0 1.1 0 | 145639. | 7.44E-06 | | 0 1.1 0 | 157774. | 9.08E-06 |
| | 0 1.1 0 | 145795. | 7.44E-06 | | 0 1.1 0 | 157943. | 9.08E-06 |
| 0.18 C.12 S.32 | 0 0.0 0 | 136908.81 | 1.45E-05 | 0.18 C.12 S.32 | 0 0.0 0 | 148316.40 | 1.77E-05 |
| | 0 1.1 0 | 137084. | 1.10E-06 | | 0 1.1 0 | 148506. | 1.34E-06 |
| | 0 1.1 0 | 137219. | 1.10E-06 | | 0 1.1 0 | 148653. | 1.34E-06 |
| 0.16 C.13 S.34 | 0 0.0 0 | 141873. | 3.88E-06 | 0.16 C.13 S.34 | 0 0.0 0 | 153694. | 4.74E-06 |
| | 0 1.1 0 | 142032. | 3.09E-07 | | 0 1.1 0 | 153866. | 3.78E-07 |
| | 0 1.1 0 | 142181. | 3.09E-07 | | 0 1.1 0 | 154027. | 3.77E-07 |
| 0.18 C.12 S.34 | 0 0.0 0 | 133432. | 5.98E-07 | 0.18 C.12 S.34 | 0 0.0 0 | 144550. | 7.30E-07 |
| | 0 1.1 0 | 133611. | 4.53E-08 | | 0 1.1 0 | 144745. | 5.54E-08 |
| | 0 1.1 0 | 133733. | 4.53E-08 | | 0 1.1 0 | 144876. | 5.54E-08 |
| 0.18 C.13 S.32 | 0 0.0 0 | 136578. | 1.59E-07 | 0.18 C.13 S.32 | 0 0.0 0 | 147958. | 1.94E-07 |
| | 0 1.1 0 | 136737. | 1.30E-08 | | 0 1.1 0 | 148130. | 1.59E-08 |
| | 0 1.1 0 | 136876. | 1.30E-08 | | 0 1.1 0 | 148281. | 1.59E-08 |
| 0.18 C.13 S.34 | 0 0.0 0 | 133069. | 6.55E-09 | 0.18 C.13 S.34 | 0 0.0 0 | 144157. | 8.00E-09 |

| J = 14 (- 13) | | | | J = 15 (- 14) | | | |
|------------------|-------------|----------------|-----------------|------------------|-------------|----------------|-----------------|
| ISOTOPIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 | ISOTOPIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 |
| 0.16 C.12 S.32 | 0 0.0 0 | 170267.50 | 1.25E-02 | 0.16 C.12 S.32 | 0 0.0 0 | 182427.20 | 1.47E-02 |
| | 0 1.1 0 | 170474.69 | 9.20E-04 | | 0 1.1 0 | 182649.15 | 1.08E-03 |
| | 0 1.1 0 | 170652.79 | 9.20E-04 | | 0 1.1 0 | 182839.97 | 1.08E-03 |
| 0.16 C.12 S.34 | 0 0.0 0 | 166105.72 | 5.17E-04 | 0.16 C.12 S.34 | 0 0.0 0 | 177968.25 | 6.08E-04 |
| | 0 1.1 0 | 166310. | 3.82E-05 | | 0 1.1 0 | 178187. | 4.50E-05 |
| | 0 1.1 0 | 166480. | 3.82E-05 | | 0 1.1 0 | 178369. | 4.50E-05 |
| 0.16 C.13 S.32 | 0 0.0 0 | 169719.65 | 1.37E-04 | 0.16 C.13 S.32 | 0 0.0 0 | 181840.22 | 1.61E-04 |
| | 0 1.1 0 | 169908. | 1.09E-05 | | 0 1.1 0 | 182042. | 1.28E-05 |
| | 0 1.1 0 | 170090. | 1.09E-05 | | 0 1.1 0 | 182237. | 1.28E-05 |
| 0.18 C.12 S.32 | 0 0.0 0 | 159723.64 | 2.12E-05 | 0.18 C.12 S.32 | 0 0.0 0 | 171130.49 | 2.50E-05 |
| | 0 1.1 0 | 159928. | 1.61E-06 | | 0 1.1 0 | 171349. | 1.89E-06 |
| | 0 1.1 0 | 160086. | 1.61E-06 | | 0 1.1 0 | 171519. | 1.89E-06 |
| 0.16 C.13 S.34 | 0 0.0 0 | 165515. | 5.67E-06 | 0.16 C.13 S.34 | 0 0.0 0 | 177335. | 6.67E-06 |
| | 0 1.1 0 | 165700. | 4.52E-07 | | 0 1.1 0 | 177534. | 5.32E-07 |
| | 0 1.1 0 | 165874. | 4.52E-07 | | 0 1.1 0 | 177720. | 5.32E-07 |
| 0.18 C.12 S.34 | 0 0.0 0 | 155667. | 8.75E-07 | 0.18 C.12 S.34 | 0 0.0 0 | 166785. | 1.03E-06 |
| | 0 1.1 0 | 155879. | 6.65E-08 | | 0 1.1 0 | 167013. | 7.84E-08 |
| | 0 1.1 0 | 156019. | 6.64E-08 | | 0 1.1 0 | 167161. | 7.84E-08 |
| 0.18 C.13 S.32 | 0 0.0 0 | 159337. | 2.33E-07 | 0.18 C.13 S.32 | 0 0.0 0 | 170717. | 2.74E-07 |
| | 0 1.1 0 | 159523. | 1.90E-08 | | 0 1.1 0 | 170916. | 2.24E-08 |
| | 0 1.1 0 | 159686. | 1.90E-08 | | 0 1.1 0 | 171090. | 2.24E-08 |
| 0.18 C.13 S.34 | 0 0.0 0 | 155244. | 9.59E-09 | 0.18 C.13 S.34 | 0 0.0 0 | 166331. | 1.13E-08 |

TABLE 7. Transitions in region $J = J' + J''$, each ordered according to frequency, for $J' = 4$ to 25 and $J'' = 3$ to 24 --Continued

| J = 16 (- 15) | | | | J = 17 (- 16) | | | |
|------------------|-------------|----------------|-----------------|------------------|-------------|----------------|-----------------|
| ISOTOPIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 | ISOTOPIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 |
| D.16 C.12 S.32 | 0 0.0 0 | 194586.43 | 1.70E-02 | O.16 C.12 S.32 | 0 0.0 0 | 206745.16 | 1.94E-02 |
| | 0 1.1 0 | 194823.14 | 1.25E-03 | | 0 1.1 0 | 206996.61 | 1.43E-03 |
| | 0 1.1 0 | 195026.67 | 1.25E-03 | | 0 1.1 0 | 207212.86 | 1.43E-03 |
| D.16 C.12 S.34 | 0 0.0 0 | 189830.33 | 7.05E-04 | O.16 C.12 S.34 | 0 0.0 0 | 201691.94 | 8.06E-04 |
| | 0 1.1 0 | 190064. | 5.22E-05 | | 0 1.1 0 | 201940. | 5.97E-05 |
| | 0 1.1 0 | 190258. | 5.22E-05 | | 0 1.1 0 | 202147. | 5.97E-05 |
| O.16 C.13 S.32 | 0 0.0 0 | 193960.32 | 1.86E-04 | O.16 C.13 S.32 | 0 0.0 0 | 206079.93 | 2.13E-04 |
| | 0 1.1 0 | 194175. | 1.48E-05 | | 0 1.1 0 | 206308. | 1.69E-05 |
| | 0 1.1 0 | 194384. | 1.48E-05 | | 0 1.1 0 | 206530. | 1.69E-05 |
| O.18 C.12 S.32 | 0 0.0 0 | 182536.94 | 2.90E-05 | O.18 C.12 S.32 | 0 0.0 0 | 193942.95 | 3.32E-05 |
| | 0 1.1 0 | 182770. | 2.20E-06 | | 0 1.1 0 | 194190. | 2.51E-06 |
| | 0 1.1 0 | 182951. | 2.20E-06 | | 0 1.1 0 | 194382. | 2.51E-06 |
| O.16 C.13 S.34 | 0 0.0 0 | 189155. | 7.73E-06 | O.16 C.13 S.34 | 0 0.0 0 | 200975. | 8.84E-06 |
| | 0 1.1 0 | 189367. | 6.17E-07 | | 0 1.1 0 | 201199. | 7.06E-07 |
| | 0 1.1 0 | 189565. | 6.17E-07 | | 0 1.1 0 | 201410. | 7.06E-07 |
| O.18 C.12 S.34 | 0 0.0 0 | 177901. | 1.20E-06 | O.18 C.12 S.34 | 0 0.0 0 | 189018. | 1.37E-06 |
| | 0 1.1 0 | 178147. | 9.10E-08 | | 0 1.1 0 | 189281. | 1.04E-07 |
| | 0 1.1 0 | 178303. | 9.10E-08 | | 0 1.1 0 | 189444. | 1.04E-07 |
| O.18 C.13 S.32 | 0 0.0 0 | 182096. | 3.18E-07 | O.18 C.13 S.32 | 0 0.0 0 | 193474. | 3.64E-07 |
| | 0 1.1 0 | 182308. | 2.60E-08 | | 0 1.1 0 | 193699. | 2.98E-08 |
| | 0 1.1 0 | 182493. | 2.60E-08 | | 0 1.1 0 | 193896. | 2.98E-08 |
| O.18 C.13 S.34 | 0 0.0 0 | 177418. | 1.31E-08 | O.18 C.13 S.34 | 0 0.0 0 | 188504. | 1.50E-08 |

| J = 18 (- 17) | | | | J = 19 (- 18) | | | |
|------------------|-------------|----------------|-----------------|------------------|-------------|----------------|-----------------|
| ISOTOPIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 | ISOTOPIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 |
| O.16 C.12 S.32 | 0 0.0 0 | 218903.36 | 2.19E-02 | O.16 C.12 S.32 | 0 0.0 0 | 231061.00 | 2.45E-02 |
| | 0 1.1 0 | 219169.55 | 1.62E-03 | | 0 1.1 0 | 231341.92 | 1.81E-03 |
| | 0 1.1 0 | 219398.52 | 1.62E-03 | | 0 1.1 0 | 231583.60 | 1.81E-03 |
| O.16 C.12 S.34 | 0 0.0 0 | 213553.03 | 9.10E-04 | O.16 C.12 S.34 | 0 0.0 0 | 225413.59 | 1.02E-03 |
| | 0 1.1 0 | 213816. | 6.74E-05 | | 0 1.1 0 | 225691. | 7.53E-05 |
| | 0 1.1 0 | 214034. | 6.74E-05 | | 0 1.1 0 | 225922. | 7.53E-05 |
| O.16 C.13 S.32 | 0 0.0 0 | 218199.00 | 2.40E-04 | O.16 C.13 S.32 | 0 0.0 0 | 230317.51 | 2.68E-04 |
| | 0 1.1 0 | 218441. | 1.91E-05 | | 0 1.1 0 | 230573. | 2.13E-05 |
| | 0 1.1 0 | 218675. | 1.91E-05 | | 0 1.1 0 | 230820. | 2.13E-05 |
| O.18 C.12 S.32 | 0 0.0 0 | 205348.50 | 3.75E-05 | O.18 C.12 S.32 | 0 0.0 0 | 216753.56 | 4.20E-05 |
| | 0 1.1 0 | 205610. | 2.84E-06 | | 0 1.1 0 | 217030. | 3.18E-06 |
| | 0 1.1 0 | 205814. | 2.84E-06 | | 0 1.1 0 | 217244. | 3.18E-06 |
| O.16 C.13 S.34 | 0 0.0 0 | 212793. | 9.98E-06 | O.16 C.13 S.34 | 0 0.0 0 | 224612. | 1.12E-05 |
| | 0 1.1 0 | 213032. | 7.98E-07 | | 0 1.1 0 | 224863. | 8.92E-07 |
| | 0 1.1 0 | 213255. | 7.97E-07 | | 0 1.1 0 | 225099. | 8.91E-07 |
| O.18 C.12 S.34 | 0 0.0 0 | 200134. | 1.55E-06 | O.18 C.12 S.34 | 0 0.0 0 | 211249. | 1.74E-06 |
| | 0 1.1 0 | 200414. | 1.18E-07 | | 0 1.1 0 | 211548. | 1.32E-07 |
| | 0 1.1 0 | 200585. | 1.18E-07 | | 0 1.1 0 | 211726. | 1.32E-07 |
| O.18 C.13 S.32 | 0 0.0 0 | 204852. | 4.11E-07 | O.18 C.13 S.32 | 0 0.0 0 | 216230. | 4.60E-07 |
| | 0 1.1 0 | 205090. | 3.37E-08 | | 0 1.1 0 | 216481. | 3.77E-08 |
| | 0 1.1 0 | 205299. | 3.37E-08 | | 0 1.1 0 | 216701. | 3.77E-08 |
| O.18 C.13 S.34 | 0 0.0 0 | 199590. | 1.70E-08 | O.18 C.13 S.34 | 0 0.0 0 | 210675. | 1.91E-08 |

TABLE 7. Transitions in regions $J = J' + J''$, each ordered according to frequency, for $J' = 4$ to 25 and $J'' = 3$ to 24--Continued

| J = 20 (- 19) | | | | J = 21 (- 20) | | | |
|-------------------|-------------|----------------|-----------------|-------------------|-------------|----------------|-----------------|
| ISOTOPIIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 | ISOTOPIIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 |
| 0.16 C.12 S.32 | 0 0.0 0 | 243218.04 | 2.71E-02 | 0.16 C.12 S.32 | 0 0.0 0 | 255374.46 | 2.96E-02 |
| | 0 1.1 0 | 243513.68 | 2.00E-03 | | 0 1.1 0 | 255684.81 | 2.19E-03 |
| | 0 1.1 0 | 243768.08 | 2.00E-03 | | 0 1.1 0 | 255951.92 | 2.19E-03 |
| 0.16 C.12 S.34 | 0 0.0 0 | 237273.58 | 1.13E-03 | 0.16 C.12 S.34 | 0 0.0 0 | 249132.98 | 1.23E-03 |
| | 0 1.1 0 | 237566. | 8.34E-05 | | 0 1.1 0 | 249440. | 9.14E-05 |
| | 0 1.1 0 | 237808. | 8.33E-05 | | 0 1.1 0 | 249694. | 9.13E-05 |
| 0.16 C.13 S.32 | 0 0.0 0 | 242435.44 | 2.96E-04 | 0.16 C.13 S.32 | 0 0.0 0 | 254552.73 | 3.24E-04 |
| | 0 1.1 0 | 242704. | 2.36E-05 | | 0 1.1 0 | 254835. | 2.58E-05 |
| | 0 1.1 0 | 242964. | 2.36E-05 | | 0 1.1 0 | 255108. | 2.58E-05 |
| 0.18 C.12 S.32 | 0 0.0 0 | 228158.10 | 4.65E-05 | 0.18 C.12 S.32 | 0 0.0 0 | 239562.09 | 5.11E-05 |
| | 0 1.1 0 | 228449. | 3.53E-06 | | 0 1.1 0 | 239867. | 3.87E-06 |
| | 0 1.1 0 | 228675. | 3.53E-06 | | 0 1.1 0 | 240104. | 3.87E-06 |
| 0.16 C.13 S.34 | 0 0.0 0 | 236430. | 1.23E-05 | 0.16 C.13 S.34 | 0 0.0 0 | 248247. | 1.35E-05 |
| | 0 1.1 0 | 236694. | 9.87E-07 | | 0 1.1 0 | 248524. | 1.08E-06 |
| | 0 1.1 0 | 236942. | 9.86E-07 | | 0 1.1 0 | 248785. | 1.08E-06 |
| 0.18 C.12 S.34 | 0 0.0 0 | 222364. | 1.93E-06 | 0.18 C.12 S.34 | 0 0.0 0 | 233479. | 2.12E-06 |
| | 0 1.1 0 | 222682. | 1.47E-07 | | 0 1.1 0 | 233815. | 1.81E-07 |
| | 0 1.1 0 | 222866. | 1.47E-07 | | 0 1.1 0 | 234005. | 1.61E-07 |
| 0.18 C.13 S.32 | 0 0.0 0 | 227607. | 5.10E-07 | 0.18 C.13 S.32 | 0 0.0 0 | 238983. | 5.60E-07 |
| | 0 1.1 0 | 227871. | 4.18E-08 | | 0 1.1 0 | 239260. | 4.59E-08 |
| | 0 1.1 0 | 228102. | 4.19E-08 | | 0 1.1 0 | 239503. | 4.59E-08 |
| 0.18 C.13 S.34 | 0 0.0 0 | 221760. | 2.11E-08 | 0.18 C.13 S.34 | 0 0.0 0 | 232844. | 2.32E-08 |
| J = 22 (- 21) | | | | J = 23 (- 22) | | | |
| ISOTOPIIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 | ISOTOPIIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 |
| 0.16 C.12 S.32 | 0 0.0 0 | 267530.22 | 3.22E-02 | 0.16 C.12 S.32 | 0 0.0 0 | 279685.30 | 3.46E-02 |
| | 0 1.1 0 | 267855.28 | 2.37E-03 | | 0 1.1 0 | 280025.04 | 2.56E-03 |
| | 0 1.1 0 | 268135.09 | 2.37E-03 | | 0 1.1 0 | 280317.57 | 2.56E-03 |
| 0.16 C.12 S.34 | 0 0.0 0 | 260991.75 | 1.34E-03 | 0.16 C.12 S.34 | 0 0.0 0 | 272849.86 | 1.44E-03 |
| | 0 1.1 0 | 261313. | 9.93E-05 | | 0 1.1 0 | 273186. | 1.07E-04 |
| | 0 1.1 0 | 261580. | 9.93E-05 | | 0 1.1 0 | 273465. | 1.07E-04 |
| 0.16 C.13 S.32 | 0 0.0 0 | 266669.38 | 3.52E-04 | 0.16 C.13 S.32 | 0 0.0 0 | 278785.34 | 3.79E-04 |
| | 0 1.1 0 | 266964. | 2.81E-05 | | 0 1.1 0 | 279094. | 3.02E-05 |
| | 0 1.1 0 | 267251. | 2.80E-05 | | 0 1.1 0 | 279393. | 3.02E-05 |
| 0.18 C.12 S.32 | 0 0.0 0 | 250965.52 | 5.56E-05 | 0.18 C.12 S.32 | 0 0.0 0 | 262368.34 | 6.00E-05 |
| | 0 1.1 0 | 251285. | 4.22E-06 | | 0 1.1 0 | 262702. | 4.55E-06 |
| | 0 1.1 0 | 251533. | 4.21E-06 | | 0 1.1 0 | 262962. | 4.55E-06 |
| 0.16 C.13 S.34 | 0 0.0 0 | 260063. | 1.47E-05 | 0.16 C.13 S.34 | 0 0.0 0 | 271879. | 1.59E-05 |
| | 0 1.1 0 | 260354. | 1.18E-06 | | 0 1.1 0 | 272183. | 1.27E-06 |
| | 0 1.1 0 | 260627. | 1.17E-06 | | 0 1.1 0 | 272468. | 1.27E-06 |
| 0.18 C.12 S.34 | 0 0.0 0 | 244593. | 2.31E-06 | 0.18 C.12 S.34 | 0 0.0 0 | 255706. | 2.49E-06 |
| | 0 1.1 0 | 244749. | 1.76E-07 | | 0 1.1 0 | 256083. | 1.90E-07 |
| | 0 1.1 0 | 245144. | 1.76E-07 | | 0 1.1 0 | 256282. | 1.90E-07 |
| 0.18 C.13 S.32 | 0 0.0 0 | 250359. | 6.09E-07 | 0.18 C.13 S.32 | 0 0.0 0 | 261734. | 6.58E-07 |
| | 0 1.1 0 | 250649. | 5.00E-08 | | 0 1.1 0 | 262037. | 5.40E-08 |
| | 0 1.1 0 | 250904. | 4.99E-08 | | 0 1.1 0 | 262303. | 5.39E-08 |
| 0.18 C.13 S.34 | 0 0.0 0 | 243728. | 2.53E-08 | 0.18 C.13 S.34 | 0 0.0 0 | 255011. | 2.74E-08 |

TABLE 7. Transitions in regions $J = J' + J''$, each ordered according to frequency, for $J' = 4$ to 25 and $J'' = 3$ to 24--Continued

| J = 24 (- 23) | | | | J = 25 (- 24) | | | |
|------------------|-------------|----------------|-----------------|------------------|-------------|----------------|-----------------|
| ISOTOPIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 | ISOTOPIC SPECIES | VIBR. STATE | FREQUENCY /MHZ | ALPHA MAX /CM-1 |
| 0.16 C.12 S.32 | 0 0.0 0 | 291839.66 | 3.70E-02 | 0.16 C.12 S.32 | 0 0.0 0 | 303993.26 | 3.93E-02 |
| | 0 1.1 0 | 292194.08 | 2.73E-03 | | 0 1.1 0 | 304362.35 | 2.90E-03 |
| | 0 1.1 0 | 292499.31 | 2.73E-03 | | 0 1.1 0 | 304680.29 | 2.90E-03 |
| 0.16 C.12 S.34 | 0 0.0 0 | 284707.28 | 1.55E-03 | 0.16 C.12 S.34 | 0 0.0 0 | 296563.99 | 1.64E-03 |
| | 0 1.1 0 | 285057. | 1.15E-04 | | 0 1.1 0 | 296929. | 1.22E-04 |
| | 0 1.1 0 | 285349. | 1.15E-04 | | 0 1.1 0 | 297232. | 1.22E-04 |
| 0.16 C.13 S.32 | 0 0.0 0 | 290900.58 | 4.06E-04 | 0.16 C.13 S.32 | 0 0.0 0 | 303015.07 | 4.31E-04 |
| | 0 1.1 0 | 291222. | 3.23E-05 | | 0 1.1 0 | 303350. | 3.43E-05 |
| | 0 1.1 0 | 291534. | 3.23E-05 | | 0 1.1 0 | 303675. | 3.43E-05 |
| 0.18 C.12 S.32 | 0 0.0 0 | 273770.54 | 6.43E-05 | 0.18 C.12 S.32 | 0 0.0 0 | 285172.08 | 6.85E-05 |
| | 0 1.1 0 | 274118. | 4.88E-06 | | 0 1.1 0 | 285534. | 5.20E-06 |
| | 0 1.1 0 | 274389. | 4.88E-06 | | 0 1.1 0 | 285816. | 5.19E-06 |
| 0.16 C.13 S.34 | 0 0.0 0 | 283695. | 1.70E-05 | 0.16 C.13 S.34 | 0 0.0 0 | 295509. | 1.80E-05 |
| | 0 1.1 0 | 284011. | 1.36E-06 | | 0 1.1 0 | 295839. | 1.44E-06 |
| | 0 1.1 0 | 284309. | 1.36E-06 | | 0 1.1 0 | 296149. | 1.44E-06 |
| 0.18 C.12 S.34 | 0 0.0 0 | 266819. | 2.68E-06 | 0.18 C.12 S.34 | 0 0.0 0 | 277931. | 2.85E-06 |
| | 0 1.1 0 | 267216. | 2.04E-07 | | 0 1.1 0 | 278349. | 2.17E-07 |
| | 0 1.1 0 | 267420. | 2.04E-07 | | 0 1.1 0 | 278557. | 2.17E-07 |
| 0.18 C.13 S.32 | 0 0.0 0 | 273109. | 7.06E-07 | 0.18 C.13 S.32 | 0 0.0 0 | 284483. | 7.51E-07 |
| | 0 1.1 0 | 273424. | 5.78E-08 | | 0 1.1 0 | 284811. | 6.16E-08 |
| | 0 1.1 0 | 273703. | 5.78E-08 | | 0 1.1 0 | 285101. | 6.16E-08 |
| 0.18 C.13 S.34 | 0 0.0 0 | 266094. | 2.94E-08 | 0.18 C.13 S.34 | 0 0.0 0 | 277176. | 3.13E-08 |

TABLE 8. NATURAL ABUNDANCE FACTORS FOR VARIOUS ISOTOPIC SPECIES OF OCS

| | |
|---|-------------------------|
| $^{16}_0\text{C}^{12}_0\text{S}^{32}_0$ | 0.937 |
| $^{16}_0\text{C}^{12}_0\text{S}^{34}_0$ | 4.163×10^{-2} |
| $^{16}_0\text{C}^{13}_0\text{S}^{32}_0$ | 1.049×10^{-2} |
| $^{18}_0\text{C}^{12}_0\text{S}^{32}_0$ | 1.1916×10^{-3} |
| $^{16}_0\text{C}^{13}_0\text{S}^{34}_0$ | 4.672×10^{-4} |
| $^{18}_0\text{C}^{12}_0\text{S}^{34}_0$ | 8.509×10^{-5} |
| $^{18}_0\text{C}^{13}_0\text{S}^{32}_0$ | 2.144×10^{-5} |
| $^{18}_0\text{C}^{13}_0\text{S}^{34}_0$ | 9.53×10^{-7} |

TABLE 9. ROTATIONAL CONSTANTS USED IN THE CALCULATION OF TRANSITION FREQUENCIES FOR VARIOUS ISOTOPIC SPECIES OF OCS

| | | B_V/MHz | D_V/kHz | q_V/MHz |
|---|----------|------------------|----------------------|------------------|
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | 00^0_0 | 6081.492475 | 1.301777 | |
| | 01^0_0 | 6092.07822 | 1.32359 | 6.3614127 |
| $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | 00^0_0 | 5932.8348 | 1.244 | |
| | 01^1_0 | 5943.1755 | 1.256 | 6.0688022 |
| $^{16}\text{O}^{13}\text{C}^{32}\text{S}$ | 00^0_0 | 6061.92510 | 1.29898 | |
| | 01^1_0 | 6071.9159 | 1.335 | 6.5078418 |
| $^{18}\text{O}^{12}\text{C}^{32}\text{S}$ | 00^0_0 | 5704.8607 | 1.1353 | |
| | 01^1_0 | 5714.995 | 1.198 | 6.6530026 |
| $^{16}\text{O}^{13}\text{C}^{34}\text{S}$ | 00^0_0 | 5911.733 | (1.241) ^a | |
| | 01^1_0 | 5921.46 | (1.267) | 6.199 |
| $^{18}\text{O}^{12}\text{C}^{34}\text{S}$ | 00^0_0 | 5559.971 | (1.078) | |
| | 01^1_0 | 5569.845 | (1.130) | 5.393 |
| $^{18}\text{O}^{13}\text{C}^{32}\text{S}$ | 00^0_0 | 5691.069 | (1.133) | |
| | 01^1_0 | 5700.627 | (1.209) | 5.800 |
| $^{18}\text{O}^{13}\text{C}^{34}\text{S}$ | 00^0_0 | 5544.864 | (1.075) | |

^a Bracketed values have been estimated, see text.

TABLE 10. COMPARISON OF THE MEASURED AND THE CALCULATED VALUES FOR PEAK ABSORPTION COEFFICIENTS IN CARBONYL SULPHIDE

| Isotopic species | Transition | $\alpha_{\text{max}}/\text{cm}^{-1}$ (measured) | Ref. | $\alpha_{\text{max}}/\text{cm}^{-1}$ (calculated ^d) |
|---|---------------------------|--|------|--|
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | $J = 2 + 1 (0\ 0^0\ 0)$ | $(5.13 \pm 0.12) \times 10^{-5}$ | a | 5.38×10^{-5} |
| | | $(5.20 \pm 0.14) \times 10^{-5}$ | b | |
| $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | $J = 2 + 1 (0\ 0^0\ 0)$ | $(2.06 \pm 0.05) \times 10^{-6}$ | a | 2.22×10^{-6} |
| $^{16}\text{O}^{13}\text{C}^{34}\text{S}$ | $J = 2 + 1 (0\ 0^0\ 0)$ | $(5.69 \pm 0.13) \times 10^{-7}$ | a | 5.89×10^{-7} |
| | | $(5.55 \pm 0.10) \times 10^{-7}$ | b | |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | $J = 2 + 1 (1\ 0^0\ 0)$ | $(7.8 \pm 0.2) \times 10^{-7}$ | a | 7.31×10^{-7} |
| | | $(8.02 \pm 0.06) \times 10^{-7}$ | b | |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | $J = 2 + 1 (0\ 1^1_1\ 0)$ | $(2.56 \pm 0.06) \times 10^{-6}$ | a | 2.99×10^{-6} |
| | | $(2.67 \pm 0.10) \times 10^{-6}$ | b | |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | $J = 2 + 1 (0\ 1^1_2\ 0)$ | $(2.54 \pm 0.06) \times 10^{-6}$ | a | 2.99×10^{-6} |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | $J = 2 + 1 (0\ 2^0\ 0)$ | $(3.06 \pm 0.08) \times 10^{-7}$ | a | 2.95×10^{-7} |
| | | $(2.97 \pm 0.10) \times 10^{-7}$ | | |
| $^{16}\text{O}^{12}\text{C}^{32}\text{S}$ | $J = 3 + 2 (0\ 0^0\ 0)$ | 2.0×10^{-4} | c | 1.78×10^{-4} |
| $^{16}\text{O}^{12}\text{C}^{34}\text{S}$ | $J = 3 + 2 (0\ 0^0\ 0)$ | 7.9×10^{-6} | c | 7.32×10^{-6} |

^a $T = 296.5\ \text{K}$, $\Delta\nu^0 = 6.40\ \text{MHz torr}^{-1}$ ref.14.

^b $T = 302\ \text{K}$, $\Delta\nu^0 = 6.12 \pm 0.03\ \text{MHz torr}^{-1}$ ref.9.

^c $T = 293\ \text{K}$, $\Delta\nu^0 = 6.3\ \text{MHz torr}^{-1}$ ref.15.

^d This work, $T = 293\ \text{K}$, $\Delta\nu^0 = 6.15$ and $6.25\ \text{MHz torr}^{-1}$ for $J = 2 + 1$ and $J = 3 + 2$ respectively.

References

- [1] Gordy, W., and Cook, R. L., *Techniques of Organic Chemistry*, Vol. IX; *Microwave Molecular Spectra*, A. Weissberger, Editor, 2nd edition, Ch. 3, p. 41, New York (1970).
- [2] Townes, C. H., and Schawlow, A. L., *Microwave Spectroscopy*, Ch. 2, p. 34, McGraw Hill, New York (1955).
- [3] Morino, Y., and Nakagawa, T., *J. Mol. Spectrosc.* **26**, 496 (1968).
- [4] Reinartz, J. M. L., and Dynamus, A., *Chem. Phys. Lett.* **24**, 346 (1974).
- [5] Tanaka, K., and Tanaka, T., *J. Mol. Spectrosc.* **69**, 335 (1978).
- [6] Jahri, G. K., and Srivastava, S. L., *Indian J. Phys. B* **51**, 23 (1977).
- [7] Cresswell, R. A., Brown, S. R., and Schwendeman, R. H., *J. Chem. Phys.* **64**, 1820 (1976).
- [8] Olson, D. S., Britt, L. O., Prakesh, V., and Boggs, J. E., *J. Phys.* **B 6**, 206 (1973).
- [9] Gilbert, J., *Rev. Sci. Instrum.* **41**, 1050 (1970).
- [10] Britt, C. O., and Boggs, J. E., *J. Chem. Phys.* **45**, 3877L (1966).
- [11] Battaglia, A., Cattani, M., and Terrini, O., *Nuovo Cimento B* **16**, 193 (1969).
- [12] Cattani, M., *J. Chem. Phys.* **52**, 4566 (1970).
- [13] Maki, A. G., *J. Phys. Chem. Ref. Data* **3**, 221 (1974).
- [14] Larsen, N. W., and Winnewisser, B. P., *Z. Naturforsch.* **29a**, 1213 (1974).
- [15] Smith, J. G., *J. Chem. Soc. Faraday Trans. II*, **72**, 2298 (1976).
- [16] Burenin, A. V., Karyakin, E. N., Krupnov, A. F., Shapin, S. M., and Val'dor, A. N., *J. Mol. Spectrosc.* **85**, 1 (1981).
- [17] Dynamus, A. J., *Physica (Utrecht)* **25**, 859 (1950).
- [18] White, W. F., NASA Technical Note D7450 (1974); cited in Kolbe, W. F., Buscher, H., and Lescovar, B., *J. Quant. Spectrosc. Radiat. Transfer*, **18**, 47 (1977).