

Microwave Spectra of Molecules of Astrophysical Interest VII. Carbon Monoxide, Carbon Monosulfide, and Silicon Monoxide

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Microwave Spectra of Molecules of Astrophysical Interest

VII. Carbon Monoxide, Carbon Monosulfide, and Silicon Monoxide

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The available data on the microwave spectra of carbon monoxide, carbon monosulfide, and silicon monoxide are critically reviewed for information applicable to radio astronomy. Molecular data such as rotational constants, centrifugal distortion parameters, dipole moments, hyperfine coupling constants, and structure are tabulated. Observed rotational transitions are presented for all measured isotopic forms of these molecules. All of the available data has been analyzed in order to predict all rotational transitions of these molecules up to 300 GHz. Error limits have been taken from the original literature for each measured transition frequency. All predicted transition frequencies are given with estimated uncertainties which represent the 90 percent confidence limit.

Key words: Carbon monoxide; carbon monosulfide; interstellar molecules; microwave spectra; molecular parameters; radio astronomy; rotational transitions; silicon monoxide.

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1. Introduction

The present tables are part of a series of critical reviews [1-6]¹ on the rotational spectra of molecules already identified in the interstellar medium. All of the available data have been gathered for each molecule and subjected to reanalysis in order to provide a consistent set of molecular constants, a check on the reliability of the measured transitions, and allow the unobserved transitions to be predicted with known uncertainty limits. Thus, the spectroscopic information presented in the following tables includes predicted as well as observed transitions in the frequency range presently accessible to the radio telescopes. The only limit invoked in the present calculations is a restriction on the maximum calculated frequency to approximately 300 GHz, which is more than sufficient to cover the frequency range of existing radio telescopes.

For the less abundant isotopic species of the molecules reported there are usually insufficient data to present a comprehensive statistical analysis of the spectrum. In these instances, reliable calculational techniques are invoked whereby molecular constants

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¹ Numbers in brackets indicate references in section 1.2.

necessary for predicting the spectrum can be determined. Details will be given in the discussion of each analysis separately. This review covers all the applicable information as of September, 1973.

A full description of the theory of rotational spectra is given in a number of texts, but the discussions by Townes and Schawlow [7] and Gordy and Cook [8] are particularly useful and the notation used here is generally consistent with these texts. The present analysis utilizes the Dunham [9] nomenclature as well as the usual spectroscopic formulation for describing the molecular parameters and energy level expressions. A general Dunham formulation of the equations for calculating the transition frequencies is

$$\nu_v = 2J[Y_{01} + Y_{11}(v + \frac{1}{2}) + Y_{21}(v + \frac{1}{2})^2] + 4J^3[Y_{02} + Y_{12}(v + \frac{1}{2})] + (6J^5 + 2J^3)Y_{03}. \quad (1)$$

The equivalent formulation in terms of the traditional spectroscopic constants is

$$\nu_v = 2JB_v - 4J^2D_v + (6J^5 + 2J^3)H_v \quad (2)$$

where $B_v = B_e - \alpha_e(v + \frac{1}{2}) + \gamma_e(v + \frac{1}{2})^2$ and $D_v = D_e + \beta_e(v + \frac{1}{2})$. Here J represents the rotational quantum number of the upper state involved in the transition, v is the vibrational quantum number, and ν is the transition frequency. The Y_{ij} are related to the traditional spectroscopic constants and are proportional to the reduced mass of the molecules as follows:

$$Y_{01} \equiv B_e \propto 1/\mu_r \quad (3a)$$

$$Y_{11} \equiv -\alpha_e \propto 1/\mu_r^{3/2} \quad (3b)$$

$$Y_{21} \equiv \gamma_e \propto 1/\mu_r^2 \quad (3c)$$

$$Y_{02} \equiv -D_e \propto 1/\mu_r^2 \quad (3d)$$

$$Y_{12} \equiv -\beta_e \propto 1/\mu_r^{5/2} \quad (3e)$$

$$Y_{03} \equiv H_e \propto 1/\mu_r^3 \quad (3f)$$

where $\mu_r = M_1M_2/(M_1 + M_2)$ with M_1 and M_2 referring to the masses of the two atoms composing the molecule. A further generalized relation which is employed in calculations for CS and SiO is known as the Kratzer relation [10]:

$$-Y_{02} = D_e = 4B_e^3/\omega_e^2 \quad (4)$$

where ω_e is the equilibrium vibrational constant for the molecule. For diatomic molecules where ω_e is sufficiently well known, this relation has been shown to be accurate to better than 1 percent.

For all of the analyses described in this review, the least squares fitting was performed utilizing a weighting

factor. This weight was equal to the inverse square of the measured uncertainty. The hyperfine structure calculations were based on the usual expression:

$$-eqQf(I, J, F) + \frac{1}{2}c[F(F+1) - J(J+1) - I(I+1)] \quad (5)$$

where $f(I, J, F)$ is the Casimir function. The values of the Casimir function as well as the calculated relative intensities for the hyperfine components can be found in Appendix I of [7]. The standard deviations quoted for both the molecular constants and predicted frequencies were selected to represent the 90 percent confidence limit. For a number of the less abundant isotopic forms, where only one transition frequency has been measured, the uncertainty in the measurement was assumed to be one standard deviation. This estimated standard deviation was then utilized in calculating the uncertainties for the predicted transitions.

Following the method of the sixth paper in this series, the present tables do not include line strengths other than the relative intensities of the nuclear electric quadrupole split transitions. The line strength, S , is a simple function of the quantum numbers as follows:

$$S(J'; J'') = J'$$

The Einstein coefficient, $A(J'; J'')$, which is the probability of a spontaneous transition in one second from the upper state, J' , to the lower state, J'' , is given by

$$A(J'; J'') = \frac{1.1639 \times 10^{-20} \nu^3 \mu^2}{2J' + 1} S(J'; J'')$$

where μ is the dipole moment in Debye and ν is the transition frequency in MHz.

1.1. List of Symbols and Conversion Factors

a. Symbols

- Y_{ij} Dunham coefficients in the power series expansion for the rotational and vibrational energy expression. (See text).
- B_v, B_e Rotational constant for the v th vibrational state (B_v) and at the equilibrium internuclear distance (B_e) respectively.

$$B_e = \frac{\hbar}{4\pi\mu_r r_e^2} [\text{MHz}]$$

- D_v, D_e Centrifugal distortion (quartic) constant. (kHz or MHz).
- H_v Sextic distortion constant. (Hz).
- eqQ Nuclear electric quadrupole coupling constant (MHz).
- c_X Spin-rotation constant related to nucleus X.

- J* Total rotational angular momentum quantum number.
- F* Total angular momentum quantum number which includes the nuclear spin for the nucleus with largest *eqQ*.
- I* Nuclear spin angular momentum quantum number.
- μ_v Dipole moment of the molecule in the *v*th vibrational state (Debye).
- v* Vibrational quantum number.
- μ_r Reduced mass (amu).
- (...) Parentheses in the numerical listings contain measured or estimated uncertainties. These should be interpreted as: 1.409(0.083) = 1.409(83) = 1.409 ± 0.083 MHz.
- and'' Prime and double prime. Superscripts to the quantum number indicators which refer to the upper and lower energy state, respectively.

b. Conversion Factors

$$Y_{01} \cong B_e \text{ (MHz)} = \frac{5.05376 \times 10^5}{\mu_r r_e^2 \text{ (amu } \text{Å}^2)}$$

$$1 \text{ cm}^{-1} = 29,979.2458 \text{ MHz}^2$$

1.2. References

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2. Carbon Monoxide

The rotational constants and other pertinent molecular parameters are given in table 1. The most extensive data available exist for $^{12}\text{C}^{16}\text{O}$, which requires only two

² In keeping with the commonly accepted convention in molecular spectroscopy, the fundamental frequencies and vibrational energies are frequently expressed in their wave-number (cm^{-1}) equivalents. The actual frequency in units of hertz may be obtained by multiplying the numbers in such tables by the speed of light expressed in centimeters per second. Energies are obtained by multiplying the frequencies by Planck's constant.

parameters for fitting, namely, B_0 and D_0 of eq (2). Since only the lowest transition, the $J=1 \leftarrow 0$, has been measured for the other isotopic species, the centrifugal distortion parameter, D_0 , had to be calculated indirectly. Here the isotopic mass dependence of D_0 as given in eq (3d) was employed. The D_0 values for all less abundant isotopic species were calculated from the D_0 value of $^{12}\text{C}^{16}\text{O}$, and the higher frequency transitions for the less abundant isotopic species were calculated from the equation:

$$\nu_{J',-J''}^i = J'(\nu_{1 \leftarrow 0}^i) - 4D_0^i(J'^3 - J'') \quad (6)$$

for $J' \geq 2$ where $\nu_{1 \leftarrow 0}^i$ is the transition frequency for $J=1 \leftarrow 0$ of the *i*th isotopic species. Because of the known breakdown in the Born-Oppenheimer approximation, which is assumed in deriving the isotopic relations given in the introduction, this technique for calculating the transition frequencies is more reliable than applying the isotope relations to B_0 . The uncertainty introduced by calculating the centrifugal distortion for the less abundant isotopic species from these isotopic relations is of the order of one part in ten thousand and, thus, relatively small in absolute terms. The uncertainties quoted for the $^{12}\text{C}^{16}\text{O}$ calculated transition frequencies in table 2 are two standard deviations, i.e., approximately 90 percent confidence limit.

Since only one measurement exists for each of the less abundant isotopic species shown in tables 3-7, it is difficult to determine the meaning of the standard deviation uncertainties quoted in terms of confidence limit. In the present analysis the reported uncertainty for the measured transition was assumed to be one standard deviation. Our experience has shown this to be generally the case. In an attempt to report the 90 percent confidence limit, three times this standard deviation was chosen.

2.1. Organization of the Spectral Tables

Tables 2 through 7 contain the rotational quantum numbers, *J*, in the first two columns. These are followed by the observed transition frequency in MHz in the third column and the calculated frequency in MHz in the fourth column. Associated with each observed or calculated frequency is the estimated uncertainty, shown in parentheses, which refers to the last digits given. The fifth column contains the upper state energy in cm^{-1} units. The last column lists the references for the observed transitions. For the convenience of the user, the transition frequencies given in tables 2-7 are listed according to increasing frequency in table 8.

2.2. Carbon Monoxide Spectral Tables

Table 1. Molecular constants for Carbon Monoxide.

Isotopic Species	B_0 (MHz)	D_0 (kHz)	Ref.
$^{12}\text{C}^{16}\text{O}$	57635.9687(26)	183.567(70)	a
$^{12}\text{C}^{17}\text{O}$	56179.9828(252)	174.388(100)	57B ^b
$^{12}\text{C}^{18}\text{O}$	54891.4239(122)	166.462(95)	58A ^b
$^{13}\text{C}^{16}\text{O}$	55101.0205(122)	167.745(96)	58A ^b
$^{13}\text{C}^{18}\text{O}$	52356.0108(122)	151.405(87)	58A ^b
$^{14}\text{C}^{16}\text{O}$	52935.8646(122)	154.786(87)	58A ^b

Dipole Moment for $^{12}\text{C}^{16}\text{O}$

$$\mu_0 = 0.112(5) \text{ [D]} \quad 58\text{B}$$

Hyperfine structure constants for $^{12}\text{C}^{17}\text{O}$

$$e q_Q(^{17}\text{O}) = 4.52(69) \text{ [MHz]}$$

$$c(^{17}\text{O}) = 24.6(106) \text{ [kHz]}$$

^aRefit to data from [57A, 58A and 70A].

^bThe $J = 1 \leftarrow 0$ transition frequencies from the references given were used in determining the B_0 values given. Note that D_0 was obtained from $^{12}\text{C}^{16}\text{O}$ value by the isotope relation, $D \propto \mu_r^{-2}$. All errors are 1 standard deviation.

Table 2. The microwave spectrum of $^{12}\text{C}^{16}\text{O}$ (MHz).

Upper State J'	Lower State J''	Transition	Observed Frequency (Est. Unc.)	Calculated Frequency (Est. Unc.) ^b	Energy Levels in cm^{-1} Upper State	Ref.
1	0	-	115271.204(5)	115271.203(5)	3.845	58A
2	1	-	230537.974(30)	230538.001(9)	11.535	57A
3	2	-	345795.989(100) ^a	345795.987(13)	23.069	70A
4	3	-	461040.811(100) ^a	461040.756(19)	38.448	70A
5	4	-	576267.934(100) ^a	576267.903(31)	57.670	70A
6	5	-	691472.978(100) ^a	691473.022(52)	80.735	70A
7	6	-	806651.719(100) ^a	806651.707(83)	107.642	70A

^aUncertainty estimated for weighting in the least squares fit.

^bIn an attempt to estimate the 90% confidence limit two standard deviations are reported.

Table 3. The microwave spectrum of $^{12}\text{C}^{17}\text{O}$ (MHz).

Transition		Observed Frequency (Est. Unc.)	Calculated Frequency (Est. Unc.) ^a	Relative Intensity	Energy Levels in cm^{-1} Upper State	Ref.
Upper State J'	Lower State J''					
1	- 0		112359.268(71)		3.748	
F = 3/2	- F = 5/2	112358.72(10)	112358.720(118)	[0.222]		57B
F = 7/2	- F = 5/2	112358.980(15)	112358.981(100)	[0.444]		57B
F = 5/2	- F = 5/2	112360.016(15)	112360.016(90)	[0.333]		57B
2	- 1		224714.351(142)		11.244	
F = 3/2	- F = 5/2		224713.51(24)	[0.040]		
F = 5/2	- F = 5/2		224714.00(16)	[0.122]		
F = 7/2	- F = 5/2		224714.14(15)	[0.171]		
F = 9/2	- F = 7/2		224714.19(15)	[0.333]		
F = 1/2	- F = 3/2		224714.71(16)	[0.067]		
F = 3/2	- F = 3/2		224714.71(15)	[0.093]		
F = 5/2	- F = 7/2		224715.03(18)	[0.016]		
F = 7/2	- F = 7/2		224715.17(20)	[0.095]		
F = 5/2	- F = 3/2		224715.29 (22)	[0.171]		
3	- 2		337061.063(210)		22.487	
F = 3/2	- F = 5/2		337060.38(26)	[0.011]		
F = 1/2	- F = 3/2		337060.59(24)	[0.011]		
F = 5/2	- F = 7/2		337060.70(24)	[0.008]		
F = 5/2	- F = 5/2		337060.84(22)	[0.066]		
F = 9/2	- F = 7/2		337060.93(21)	[0.194]		
F = 3/2	- F = 3/2		337060.96(22)	[0.055]		
F = 11/2	- F = 9/2		337060.95(21)	[0.286]		
F = 7/2	- F = 7/2		337061.04(21)	[0.065]		
F = 1/2	- F = 1/2		337061.14(21)	[0.037]		
F = 7/2	- F = 5/2		337061.18(21)	[0.122]		
F = 5/2	- F = 3/2		337061.10(22)	[0.069]		
F = 3/2	- F = 1/2		337061.51(22)	[0.030]		
F = 9/2	- F = 9/2		337061.91(25)	[0.044]		
F = 7/2	- F = 9/2		337062.02(26)	[0.004]		

^aThe three standard deviations reported are expected to approximate the 90% confidence limit.

Table 4. The microwave spectrum of $^{12}\text{C}^{18}\text{O}$ (MHz).

Transition		Observed Frequency (Est. Unc.)	Calculated Frequency (Est. Unc.)	Energy Levels in cm^{-1} Upper State	Ref.
Upper State J'	Lower State J''				
1	- 0	109782.182(8)	109782.182(24) ^a	3.662	58A
2	- 1		219560.369(50)	10.986	
3	- 2		329330.566(81)	21.971	

^aThe uncertainty assigned is 3 times that of the measured frequency. Under the assumption that the measurement uncertainty is one standard deviation, the calculated uncertainties represent the 90% confidence limit.

Table 5. The microwave spectrum of $^{13}\text{C}^{16}\text{O}$ (MHz).

Transition		Observed Frequency (Est. Unc.)	Calculated Frequency (Est. Unc.)	Energy Levels in cm^{-1} Upper State	Ref.
Upper State J'	Lower State J''				
1	- 0	110201.370(8)	110201.370(24) ^a	3.676	58A
2	- 1		220398.714(50)	11.028	
3	- 2		330588.006(81)	22.055	

^aThe uncertainty assigned is 3 times that of the measured frequency. Under the assumption that the measurement uncertainty is one standard deviation, the calculated uncertainties represent the 90% confidence limit.

Table 6. The microwave spectrum of $^{13}\text{C}^{18}\text{O}$ (MHz).

Transition		Observed Frequency (Est. Unc.)	Calculated Frequency (Est. Unc.)	Energy Levels in cm^{-1} Upper State	Ref.
Upper State J'	Lower State J''				
1	- 0	104711.416(8)	104711.416(24) ^a	3.493	58A
2	- 1		209419.198(50)	10.478	
3	- 2		314119.713(80)	20.956	

^aThe uncertainty assigned is 3 times that of the measured frequency. Under the assumption that the measurement uncertainty is one standard deviation, the calculated uncertainties represent the 90% confidence limit.

Table 7. The microwave spectrum of $^{14}\text{C}^{16}\text{O}$ (MHz).

Transition		Observed Frequency (Est. Unc.)	Calculated Frequency (Est. Unc.)	Energy Levels in cm^{-1} Upper State	Ref.
Upper State J'	Lower State J''				
1	- 0	105871.110(4)	105871.110(24) ^a	3.531	58A
2	- 1		211738.505(50)	10.594	
3	- 2		317598.471(80)	21.188	

^aThe uncertainty assigned is 6 times that of the measured frequency. Under the assumption that the measurement uncertainty is one standard deviation, the calculated uncertainties represent the 90% confidence limit.

Table 8. Calculated microwave transitions in CO
in order of frequency (MHz).

Calculated Frequency	Isotopic Species	Transition $J' - J''$	Estimated Uncertainty
104711.416	$^{13}\text{C}^{18}\text{O}$	1 - 0	(0.024)
105871.110	$^{14}\text{C}^{16}\text{O}$	1 - 0	(0.024)
109782.182	$^{12}\text{C}^{18}\text{O}$	1 - 0	(0.024)
110201.370	$^{13}\text{C}^{16}\text{O}$	1 - 0	(0.024)
112359.268	$^{12}\text{C}^{17}\text{O}$	1 - 0	(0.071)
115271.203	$^{12}\text{C}^{16}\text{O}$	1 - 0	(0.005)
209419.198	$^{13}\text{C}^{18}\text{O}$	2 - 1	(0.050)
211738.505	$^{14}\text{C}^{16}\text{O}$	2 - 1	(0.050)
219560.369	$^{12}\text{C}^{18}\text{O}$	2 - 1	(0.050)
220398.714	$^{13}\text{C}^{16}\text{O}$	2 - 1	(0.050)
224714.351	$^{12}\text{C}^{17}\text{O}$	2 - 1	(0.142)
230538.001	$^{12}\text{C}^{16}\text{O}$	2 - 1	(0.009)
314119.713	$^{13}\text{C}^{18}\text{O}$	3 - 2	(0.080)
317598.471	$^{14}\text{C}^{16}\text{O}$	3 - 2	(0.080)
329330.566	$^{12}\text{C}^{18}\text{O}$	3 - 2	(0.081)
330588.006	$^{13}\text{C}^{16}\text{O}$	3 - 2	(0.081)
337061.063	$^{12}\text{C}^{17}\text{O}$	3 - 2	(0.210)
345795.987	$^{12}\text{C}^{16}\text{O}$	3 - 2	(0.013)
461040.756	$^{12}\text{C}^{16}\text{O}$	4 - 3	(0.019)
576267.903	$^{12}\text{C}^{16}\text{O}$	5 - 4	(0.031)
691473.022	$^{12}\text{C}^{16}\text{O}$	6 - 5	(0.052)
806651.707	$^{12}\text{C}^{16}\text{O}$	7 - 6	(0.083)

2.3. CO References

a. Laboratory References

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b. Interstellar References

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3. Carbon Monosulfide

The present reanalysis of the rotational spectrum of $^{12}\text{C}^{32}\text{S}$ and $^{12}\text{C}^{34}\text{S}$ differs from that given in the most

recent source of data [63A] in that we find B_0 and D_0 as the determinable parameters. In [63A], the parameters B_0 , D_0 and H_0 from eq (2) were used in fitting the available data. The present analysis shown in table 9 utilizes only B_0 and D_0 , since it was concluded that H_0 was not a determinable constant. The standard deviation errors shown represent the 90 percent confidence limit.

In the case of $^{12}\text{C}^{32}\text{S}$ where five of the six rotational transitions have been measured, a least squares fit which includes H_0 produced the following constants:

$$\begin{aligned} B_0 &= 24495.586(5) \text{ MHz}, \\ D_0 &= 42.18(70) \text{ kHz}, \\ H_0 &= 50.54(18) \text{ Hz}, \end{aligned}$$

quoting two standard deviation errors. Here the magnitude of H_0 seems much greater than expected from several points of view. First of all, a generally applicable approximation: $D_e/H_e \cong \omega_e^2/B_e^2 = 10^6$ indicates that H_0 should be 0.04 Hz rather than 50 Hz. In addition, there is another approximation for estimating H_e from the value of α_e :

$$H_e = -8/3 (B_e^3/\omega_e^3)\alpha_e + 32 B_e^5/\omega_e^4.$$

Since the $J=1 \leftarrow 0$, $v=1$ transition for $^{12}\text{C}^{32}\text{S}$ has been measured, $\nu = 48635.912(40)$, a value of $\alpha_e = 177.54(3)$ [55A], can be determined and thereby H_e is estimated from the above relation to be +0.01 Hz. Values of H_0 of this magnitude would contribute less than 2 kHz to the $J=5-4$ transition, two orders of magnitude smaller than the measurement uncertainty. A further point of comparison is possible. Since three transitions of $^{12}\text{C}^{34}\text{S}$ have been observed, B_0 and D_0 can be derived with reasonable accuracy. Via the isotope relation, eq (3d), applied to D_0 for $^{12}\text{C}^{32}\text{S}$, a value of D_0 ($^{12}\text{C}^{34}\text{S}$) = 34.96(54) kHz is obtained. This D_0 value agrees well with that derived for $^{12}\text{C}^{34}\text{S}$ from the transition frequencies as shown

in table 9 where the six standard deviation error shown represent the 90 percent confidence limit. In order to make the final comparison, an over-determined fit of three parameters B_0 , D_0 and H_0 , to the three transitions was carried out with the results

$$\begin{aligned} B_0 &= 24103.553 \text{ MHz}, \\ D_0 &= 39.792 \text{ kHz}, \\ H_0 &= 62.5 \text{ Hz}, \end{aligned}$$

wherein no estimated uncertainty can be given due to zero degrees of freedom in the fit. Note that not only is H_0 again unreasonably large, but D_0 is calculated 1 kHz larger than the two calculations described above. For these reasons the H_0 values appear to be misleading and undeterminable from the data available.

Calculations of the remaining two isotopic species of CS, namely $^{12}\text{C}^{33}\text{S}$ and $^{13}\text{C}^{32}\text{S}$ followed the procedure employed for most of the CO calculations. Since only the $J=1-0$ transitions have been observed, D_0 was computed via the isotope relations. The transition frequencies were then calculated according to eq (6) in order to minimize the estimated uncertainties. Since the hyperfine structure calculation was overdetermined for $^{12}\text{C}^{33}\text{S}$ following eq (5), the quoted uncertainties are four standard deviations while those for $^{13}\text{C}^{32}\text{S}$ are two standard deviations. All uncertainties are expected to represent the 90 percent confidence limit.

3.1. Organization of the Spectral Tables

Following the format of the CO tables as well as those of earlier reviews in this series, the format of tables 10 through 13 contain, first the quantum numbers, then the observed transition frequency, the calculated frequency and estimated uncertainty in parentheses, the energy of the upper state and finally references to measurements. Table 14 contains all the CS transitions up to 300 GHz, listed according to increasing frequency.

3.2. Carbon Monosulfide Spectral Tables

Table 9. Molecular constants for Carbon Monosulfide.

Constant ^a	$^{12}\text{C}^{32}\text{S}$	$^{12}\text{C}^{33}\text{S}$	$^{12}\text{C}^{34}\text{S}$	$^{13}\text{C}^{32}\text{S}$
B_0 (MHz)	24495.5746(102)	24293.3390(63)	24103.5507(121)	23123.808(20)
D_0 (kHz)	40.237(568)	39.574(559) ^b	38.774(776)	35.849(506) ^b
eqQ [^{33}S] (MHz)		12.835(33)		
c_s (kHz)		18.7(37)		
μ_0 (Debye)	1.958(5) ^c			

^aThe constants were derived from the data in references [63A] and [55A] unless otherwise indicated. $^{12}\text{C}^{32}\text{S}$: Uncertainty in B_0 and D_0 represents 2 standard deviation, based on a least squares fit with 3 degrees of freedom; uncertainty in μ_0 is 1 standard deviation. $^{12}\text{C}^{33}\text{S}$: Uncertainty in B_0 and D_0 represents 2 standard deviation; uncertainty in eqQ and c_s represents 1 standard deviation; $^{12}\text{C}^{34}\text{S}$: Uncertainty in B_0 and D_0 represents 6 standard deviation, based on a least squares fit with 1 degree of freedom. $^{13}\text{C}^{32}\text{S}$: Uncertainty in B_0 and D_0 represents 2 standard deviation.

^bCalculated from the D_0 value for $^{12}\text{C}^{32}\text{S}$ by use of the isotope relation.

^cReference [68A].

Table 10. The microwave spectrum of $^{12}\text{C}^{32}\text{S}$ (MHz).

Transition		Observed Frequency ^a	Calculated Frequency ^b	Energy Levels	Ref.
Upper state J'	Lower state J''	(Est. Unc.)	(Est. Unc.)	in cm^{-1} Upper state	
1	- 0	48991.000(12)	48990.988(20)	1.634	55A
2	- 1	97981.007(16)	97981.011(32)	4.902	63A
3	- 2	146969.039(60)	146969.102(50)	9.804	63A
4	- 3	195954.162(100)	195954.296(108)	16.340	63A
5	- 4	244935.737(100)	244935.627(226)	24.510	63A
6	- 5		293912.13(42)	34.314	

^a Estimated uncertainty represents 1 standard deviation.

^b In an attempt to estimate the 90% confidence limit two standard deviations are reported.

Table 11. The microwave spectrum of $^{12}\text{C}^{33}\text{S}$ (MHz).

Transition		Observed Frequency ^a	Calculated Frequency ^b	Relative Intensity ^c	Energy Levels	Ref.
Upper state J'	Lower state J''	(Est. Unc.)	(Est. Unc.)		in cm^{-1} Upper State	
1	0		48586.5107(248)		1.621	
F = 1/2	- F = 3/2	48583.264(10)	48583.264(25)	[0.167]		55A
F = 5/2	- F = 3/2	48585.906(10)	48585.906(25)	[0.500]		55A
F = 3/2	- F = 3/2	48589.068(10)	48589.068(25)	[0.333]		55A
2	- 1		97172.090(56)		4.862	
F = 1/2	- F = 3/2		97166.239(100)	[0.017]		
F = 3/2	- F = 3/2		97169.486(68)	[0.107]		
F = 5/2	- F = 3/2		97171.824(56)	[0.210]		
F = 7/2	- F = 5/2		97171.843(60)	[0.400]		
F = 1/2	- F = 1/2		97172.053(64)	[0.083]		
F = 3/2	- F = 5/2		97172.648(80)	[0.010]		
F = 5/2	- F = 5/2		97175.042(66)	[0.090]		
F = 3/2	- F = 1/2		97175.289(66)	[0.083]		
3	- 2		145755.760(130)		9.725	
F = 3/2	- F = 3/2		145753.137(140)	[0.040]		
F = 5/2	- F = 5/2		145754.054(140)	[0.052]		
F = 7/2	- F = 5/2		145755.617(132)	[0.245]		
F = 9/2	- F = 7/2		145755.635(132)	[0.359]		
F = 3/2	- F = 1/2		145756.374(132)	[0.100]		
F = 5/2	- F = 3/2		145756.392(132)	[0.160]		
F = 7/2	- F = 7/2		145758.760(140)	[0.041]		
4	- 3		194336.582(286)		16.207	
F = 5/2	- F = 5/2		194334.573(294)	[0.073]		
F = 7/2	- F = 7/2		194335.285(292)	[0.030]		
F = 9/2	- F = 7/2		194336.495(286)	[0.255]		
F = 11/2	- F = 9/2		194336.513(286)	[0.333]		
F = 5/2	- F = 3/2		194336.829(286)	[0.143]		
F = 7/2	- F = 5/2		194336.848(286)	[0.191]		
F = 9/2	- F = 9/2		194339.619(294)	[0.023]		
5	- 4		242913.605(550)		24.310	
F = 11/2	- F = 9/2		242913.547(550)	[0.258]		
F = 13/2	- F = 11/2		242913.566(550)	[0.318]		
F = 7/2	- F = 5/2		242913.730(550)	[0.167]		
F = 9/2	- F = 7/2		242913.748(550)	[0.207]		
6	- 5		291485.879(950)		34.033	

Table 11. The microwave spectrum of $^{12}_{12}\text{C}^{33}\text{S}$ (MHz)—Continued

Transition		Observed Frequency ^a (Est. Unc.)	Calculated Frequency ^b (Est. Unc.)	Relative Intensity ^c	Energy Levels in cm^{-1} Upper State	Ref.
Upper state J'	Lower state J''					
F = 13/2	- F = 11/2		291485.839(950)	[0.259]		
F = 15/2	- F = 13/2		291485.858(950)	[0.308]		
F = 9/2	- F = 7/2		291485.948(950)	[0.182]		
F = 11/2	- F = 9/2		291485.967(950)	[0.217]		

^aEstimated uncertainty is approximately 1 standard deviation.

^bEstimated uncertainty is 4 standard deviations, in an attempt to estimate the 90% confidence limit.

^cWith the exception of the J = 2 - 1 hyperfine structure calculations for which all allowed transitions are included, the calculated transitions were limited to those with relative intensities greater than 0.01 or one percent. The relative intensities are based on unity for each rotational transition J' - J''.

Table 12. The microwave spectrum of $^{12}_{12}\text{C}^{34}\text{S}$ (MHz).

Transition		Observed Frequency ^a (Est. Unc.)	Calculated Frequency ^b (Est. Unc.)	Energy Levels in cm^{-1} Upper state	Ref.
Upper state J'	Lower state J''				
1	- 0	48206.948(12)	48206.946(22)	1.608	55A
2	- 1	96412.953(30)	96412.962(28)	4.824	63A
3	- 2	144617.117(16)	144617.116(32)	9.648	63A
4	- 3		192818.48(11)	16.080	
5	- 4		241016.12(28)	24.119	
6	- 5		289209.11(53)	33.766	

^aEstimated uncertainty represents 1 standard deviation.

^bEstimated uncertainty represents 6 standard deviations, in an attempt to estimate the 90% confidence limit.

Table 13. The microwave spectrum of $^{13}_{13}\text{C}^{32}\text{S}$ (MHz).

Transition		Observed Frequency ^b (Est. Unc.)	Calculated Frequency ^c (Est. Unc.)	Energy Levels in cm^{-1} Upper state	Ref.
Upper state J'	Lower state J''				
1	- 0	46247.472(20)	46247.472(40) ^a	1.543	55A
2	- 1		92494.084(81)	4.628	
3	- 2		138738.97(13)	9.256	
4	- 3		184981.28(20)	15.426	
5	- 4		231220.15(31)	23.139	
6	- 5		277454.72(49)	32.394	

^aAll predicted transition frequencies are based on this value, using the D_0 value from $^{12}_{12}\text{C}^{32}\text{S}$ and the isotope relations.

^bEstimated uncertainty represents 1 standard deviation.

^cEstimated uncertainty represents 2 standard deviations, in an attempt to estimate the 90% confidence limit.

Table 14. Calculated microwave transitions in CS in order of frequency (MHz).

Calculated Frequency	Isotopic Species	Transition $J' - J''$	(Est. Unc)
46247.472	$^{13}\text{C}^{32}\text{S}$	1 - 0	(0.040)
48206.946	$^{12}\text{C}^{34}\text{S}$	1 - 0	(0.022)
48586.5197 ^a	$^{12}\text{C}^{33}\text{S}$	1 - 0	(0.0248)
48990.988	$^{12}\text{C}^{32}\text{S}$	1 - 0	(0.020)
92494.084	$^{13}\text{C}^{32}\text{S}$	2 - 1	(0.081)
96412.962	$^{12}\text{C}^{34}\text{S}$	2 - 1	(0.028)
97172.090 ^a	$^{12}\text{C}^{33}\text{S}$	2 - 1	(0.056)
97981.011	$^{12}\text{C}^{32}\text{S}$	2 - 1	(0.032)
138738.97	$^{13}\text{C}^{32}\text{S}$	3 - 2	(0.13)
144617.116	$^{12}\text{C}^{34}\text{S}$	3 - 2	(0.032)
145755.760 ^a	$^{12}\text{C}^{33}\text{S}$	3 - 2	(0.130)
146969.102	$^{12}\text{C}^{32}\text{S}$	3 - 2	(0.050)
184981.28	$^{13}\text{C}^{32}\text{S}$	4 - 3	(0.20)
192818.48	$^{12}\text{C}^{34}\text{S}$	4 - 3	(0.11)
194336.58 ^a	$^{12}\text{C}^{33}\text{S}$	4 - 3	(0.29)
195954.30	$^{12}\text{C}^{32}\text{S}$	4 - 3	(0.11)
231220.15	$^{13}\text{C}^{32}\text{S}$	5 - 4	(0.31)
241016.12	$^{12}\text{C}^{34}\text{S}$	5 - 4	(0.28)
242913.61 ^c	$^{12}\text{C}^{33}\text{S}$	5 - 4	(0.55)
244935.63	$^{12}\text{C}^{32}\text{S}$	5 - 4	(0.23)
277454.72	$^{13}\text{C}^{32}\text{S}$	6 - 5	(0.49)
289209.11	$^{12}\text{C}^{34}\text{S}$	6 - 5	(0.53)
291485.88 ^a	$^{12}\text{C}^{33}\text{S}$	6 - 5	(0.95)
293912.13	$^{12}\text{C}^{32}\text{S}$	6 - 5	(0.42)

^aCalculated hypothetical rotational transition frequency. See table 11 for transition frequencies including the hyperfine splittings.

3.3. CS References

a. Laboratory References

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4. Silicon Monoxide

The reanalysis of SiO was carried out in two fashions. Both methods employ Y_{02} (D_0) calculated according to eq (4) with $\omega_e = 1241.4 \text{ cm}^{-1}$ [52A], since only the $J=1 \leftarrow 0$ transitions have been measured. The first calculation followed that discussed for several of the CO and CS isotopic species, whereby eq (6) was used with the $J=1 \leftarrow 0$, $v=0$ measured frequencies. In addition, since the Born-Oppenheimer approximation appears to hold to the accuracy of these measurements, all these isotopic forms of SiO were fit simultaneously by means of the isotope relations in eq (3). The second procedure, which was used for the final calculations reported in tables 15 to 19, followed the method described above, but also included the measured $^{28}\text{Si}^{16}\text{O}$ $J=1 \leftarrow 0$ transitions for the excited vibrational states. The results from both methods were in good agreement. The second method was selected for the final results, since it accounts for all the data available. The reanalysis given in table 15 produced nearly identical results to those reported by Törring [68A]. One minor difference occurs in the Y_{02} (D_0) values employed, but the difference is well within the estimated uncertainties.

The estimated uncertainties were based on assuming a 1 percent model error in eq (4), used in deriving Y_{02} , to be equivalent to one standard deviation. Since all transitions were measured with equivalent accuracy, the fitting was carried out with uniform weighting. All constants and predicted transitions are reported with three standard deviation uncertainties in an attempt to estimate the 90 percent confidence limit.

4.1. Organization of the Spectral Tables

Tables 16, 17, and 18 contain the observed and predicted rotational transition frequencies of SiO. Since

the table format is identical to those of CO and CS, refer to sections 2.2 and 3.2 for a complete description. Table 19 contains the SiO transition frequencies ordered according to increasing frequency.

4.2. Silicon Monoxide Spectral Tables

Table 15. Molecular constants for Silicon Monoxide.

	$^{28}\text{Si}^{16}\text{O}$	$^{29}\text{Si}^{16}\text{O}$	$^{30}\text{Si}^{16}\text{O}$	Ref.
Y_{01} [MHz]	21787.459(75)	21514.070(75)	21259.479(75)	a
Y_{11} [MHz]	-151.048(114)	-148.214(114)	-145.591(114)	a
Y_{21} [MHz]	0.0762(30)	0.0743(30)	0.0726(30)	a
$Y_{02}(\equiv -D_e)$ [kHz]	-29.87(30)	-29.113(30)	-28.44(30)	b
μ_0 [D]	3.0982(10)			70A

^aRefit to data from [68A] with 3 standard deviation errors quoted. The present results are nearly identical to those in [68A].

^bCalculated from $\omega_e = 1241.4_4 \text{ cm}^{-1}$ [52A] using Kratzer's relation.

Table 16. The microwave spectrum of $^{28}\text{Si}^{16}\text{O}$ (MHz).

Transition			Vib.	Observed Frequency	Calculated Frequency ^a	Energy Levels	Ref.
Upper State	Lower State		State	(Est. Unc.)	(Est. Unc.)	in cm^{-1}	
J'	-	J''	v			Upper State	
1	-	0	0	43423.76(10)	43423.788(78)	1.448	68A
1	-	0	1	43122.03(10)	43121.998(99)	1231.0	68A
1	-	0	2	42820.48(10)	42820.510(99)	2448.8	68A
1	-	0	3	42519.34(10)	42519.328(131)	3654.7	68A
2	-	1	0		86846.859(182)	4.345	
3	-	2	0		130268.49(32)	8.690	
4	-	3	0		173687.98(53)	14.484	
5	-	4	0		217104.61(83)	21.726	
6	-	5	0		260517.64(117)	30.416	
7	-	6	0		303926.37(175)	40.554	

^aThe estimated uncertainty is 3 standard deviations, in an attempt to estimate the 90% confidence limit.

Table 17. The microwave spectrum of $^{29}\text{Si}^{16}\text{O}$ in the ground vibrational state (MHz).

Transition			Observed Frequency	Calculated Frequency ^a	Energy Levels	Ref.
Upper State	Lower State		(Est. Unc.)	(Est. Unc.)	in cm^{-1}	
J'	-	J''			Upper State	
1	-	0	42879.82(10)	42879.846(78)	1.430	68A
2	-	1		85758.997(180)	4.291	
3	-	2		128636.74(32)	8.582	
4	-	3		171512.40(53)	14.308	
5	-	4		214385.26(83)	21.454	
6	-	5		257254.61(117)	30.035	
7	-	6		300119.77(175)	40.046	

^aThe estimated uncertainty is 3 standard deviations, in attempt to estimate the 90% confidence limit.

Table 18. The microwave spectrum of $^{30}\text{Si}^{16}\text{O}$ in the ground vibrational state (MHz).

Transition		Observed Frequency (Est. Unc.)	Calculated Frequency ^a (Est. Unc.)	Energy Levels in cm^{-1} Upper State	Ref.
Upper State J'	Lower State J''				
1	- 0	42373.34(10)	42373.290(77)	1.413	68A
2	- 1		84745.898(179)	4.240	
3	- 2		127117.14(32)	8.480	
4	- 3		169486.33(53)	14.134	
5	- 4		211852.79(83)	21.201	
6	- 5		254215.86(117)	29.680	
7	- 6		296574.80(175)	39.573	

^aThe estimated uncertainty is 3 standard deviations, in an attempt to estimate the 90% confidence limit.

Table 19. Calculated microwave transitions in SiO

in order of frequency (MHz)

Calculated Frequency ^a	Isotopic Species	Transition J' - J''	Estimated Uncertainty
42373.290	$^{30}\text{Si}^{16}\text{O}$	1 - 0	(0.077)
42879.846	$^{29}\text{Si}^{16}\text{O}$	1 - 0	(0.078)
43423.788	$^{28}\text{Si}^{16}\text{O}$	1 - 0	(0.078)
84745.898	$^{30}\text{Si}^{16}\text{O}$	2 - 1	(0.179)
85758.997	$^{29}\text{Si}^{16}\text{O}$	2 - 1	(0.180)
86846.859	$^{28}\text{Si}^{16}\text{O}$	2 - 1	(0.182)
127117.14	$^{30}\text{Si}^{16}\text{O}$	3 - 2	(0.32)
128636.74	$^{29}\text{Si}^{16}\text{O}$	3 - 2	(0.32)
130268.49	$^{28}\text{Si}^{16}\text{O}$	3 - 2	(0.32)
169486.33	$^{30}\text{Si}^{16}\text{O}$	4 - 3	(0.53)
171512.40	$^{29}\text{Si}^{16}\text{O}$	4 - 3	(0.53)
173687.98	$^{28}\text{Si}^{16}\text{O}$	4 - 3	(0.53)
211052.79	$^{30}\text{Si}^{16}\text{O}$	5 - 4	(0.83)
214385.25	$^{29}\text{Si}^{16}\text{O}$	5 - 4	(0.83)
217104.61	$^{28}\text{Si}^{16}\text{O}$	5 - 4	(0.83)
254215.86	$^{30}\text{Si}^{16}\text{O}$	6 - 5	(1.17)
257254.61	$^{29}\text{Si}^{16}\text{O}$	6 - 5	(1.17)
260517.64	$^{28}\text{Si}^{16}\text{O}$	6 - 5	(1.17)
296574.80	$^{30}\text{Si}^{16}\text{O}$	7 - 6	(1.75)
300119.77	$^{29}\text{Si}^{16}\text{O}$	7 - 6	(1.75)
303926.37	$^{28}\text{Si}^{16}\text{O}$	7 - 6	(1.75)

^aOnly the transitions for SiO in the ground vibrational state are included although 3 transitions of $^{28}\text{Si}^{16}\text{O}$ in excited vibrational states are in the analysis.

4.3. SiO References

a. Laboratory References

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b. Interstellar References

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