

Microwave Spectra of Molecules of Astrophysical Interest

VIII. Sulfur Monoxide

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The available data on the microwave spectrum of sulfur monoxide (SO) is critically reviewed and tabulated. Molecular data such as rotational constants, hyperfine coupling constants, electric dipole moment, and magnetic g-factors are given. All rotational transitions up to 350 GHz for the isotopic species $^{32}\text{S}^{16}\text{O}$, $^{34}\text{S}^{16}\text{O}$, and $^{32}\text{S}^{18}\text{O}$ in the ground vibrational state are calculated and tabulated along with their estimated 95 percent confidence levels. The line strengths of all tabulated transitions have been determined. A bibliography of SO is given which includes results from microwave spectroscopy as well as from electron paramagnetic resonance.

Key words: Interstellar molecules; microwave spectra; molecular parameters; radio astronomy; rotational transitions; spectra; sulfur monoxide.

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1. Introduction

The present tables are part of a series of critical reviews which are intended to update and revise the existing tabulated literature on the microwave spectra of molecules already identified by interstellar observations. This review may also be useful to other workers since all measurements with microwave spectroscopy and electron paramagnetic resonance on SO are included. This review covers all information available as of September 1, 1973.

1.1. Molecular Parameter Tables

The theory of the rotational spectrum of a $^3\Sigma$ diatomic molecule has been described by several au-

thors. In this review the formulation by Tischer [1]¹ was used because this formulation provides the most complete centrifugal distortion analysis for $^3\Sigma$ molecules at this time. A discussion of the molecular parameters can be found in Tinkham and Strandberg [2] and Kayama and Baird [3].

Although the hyperfine structure in $^3\Sigma$ molecules has been outlined by Frosch and Foley [4], the hyperfine coupling constants of $^{33}\text{S}^{16}\text{O}$ were actually evaluated using the approximation of Amano et al. [5]. Wherever possible the experimental data were combined in a least-squares analysis in which each measurement was weighted by the inverse square of its estimated uncertainty. In all cases the available data were insufficient to form a firm statistical basis for estimating the reliability of the rotational constants and the resulting transitions calculated from those constants. Therefore, the uncertainties were estimated in a more subjective fashion from the un-

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¹ Numbers in brackets indicate references in section 1.2.

certainties given for the measurements and the limitation of the theoretical model caused by the neglect of higher order terms. The uncertainties listed in the tables are expected to be equivalent to a 95 percent confidence level. The molecular constants given in the tables are quoted with an adequate number of significant figures to allow one to reproduce the original fit to the observed transitions without reduction in accuracy due to round-off.

The molecular constants of $^{32}\text{S}^{18}\text{O}$ shown in table 1 were calculated by using isotopic relations for λ_0 , γ_0 and D_0 to transfer these values from the isotope $^{32}\text{S}^{16}\text{O}$ and then by fitting the observed spectrum to the parameter B_0 and ρ_0 . This procedure was necessary because the data available for this species are not precise enough to give better values for the constants λ_0 and γ_0 due to the strong correlation in the observed transitions. For $^{33}\text{S}^{16}\text{O}$ all rotational constants were calculated with isotopic relations from $^{32}\text{S}^{16}\text{O}$ and the hyperfine constants were fitted to the observed spectral splittings.

1.2. Microwave Spectral Tables

Tables 4, 5, and 6 contain both observed and calculated rotational transitions for the isotopic forms $^{32}\text{S}^{16}\text{O}$, $^{34}\text{S}^{16}\text{O}$ and $^{32}\text{S}^{18}\text{O}$ in the ground vibrational state. These tables also give the energy in cm^{-1} of both the upper and lower states involved in each transition. The cut-off frequency for the transitions included in these tables was chosen at 350 GHz. It is felt that this limit is generous enough to allow for the presentation of all transitions which might be observed in the relatively near future. The prediction of transitions at higher frequencies with the available molecular parameters would result in large uncertainties in most cases. The stated uncertainties represent 95 percent confidence levels.

The rotational levels are characterized by the quantum number J for the total angular momentum and the quantum number K which represents the rotational angular momentum of the molecule in the pure Hund's coupling case *b*, but which is only an approximate quantum number for the intermediate case of the SO molecule. The spin-spin interaction, λ , produces a mixing of the states $K=J+1$ and $K=J-1$ for the same total angular momentum J . The allowed electric dipole transitions are given by the selection rules $\Delta K=\pm 1$ and $\Delta J=0, \pm 1$ in the pure Hund's coupling case *b*. Only transitions which obey these selection rules have been observed in the laboratory.

The line strengths given in tables 4, 5, and 6 were calculated taking the intermediate coupling case between Hund's case *a* and *b* for SO into account. The line strength, denoted by $S(J', K'; J'', K'')$, is defined in this review as

$$S(J', K'; J'', K'') = \frac{(2J''+1) |\mu_{J' \leftarrow J''}|^2}{\mu},$$

where $|\mu_{J' \leftarrow J''}|^2$ is the square of the dipole moment matrix element connecting the upper, J' , K' , and the lower, J'' , K'' , rotational levels, and μ is the magnitude of the electric dipole moment. Thus the line strength as defined above is independent of the absolute magnitude of the dipole moment.

For transitions in which K values higher than 8 are involved, the line strengths of pure Hund's coupling case *b* can be used. For SO this approximation gives line strengths which are accurate to better than 1 percent or 0.05 in the absolute value, whichever is greater. In Hund's coupling case *b* the line strengths for $^3\Sigma$ molecules are:

$$S(J, K; J-1, K-1) = \frac{(K+J+2) (K+J+1) (K+J-1) (K+J-2)}{4J(2K+1) (2K-1)},$$

$$S(J, K; J, K-1) = \frac{(K+J+2) (K+J-1) (K-J+1) (K-J-2) (2J+1)}{4J(J+1) (2K+1) (2K-1)},$$

$$S(J, K; J+1, K-1) = \frac{(K-J+1) (K-J) (K-J-2) (K-J-3)}{4(J+1) (2K+1) (2K-1)}.$$

Transitions with $\Delta K=0$ and ± 2 are only allowed for magnetic dipole transitions, which are not listed in this review. The transitions $\Delta K=3$, which are allowed electric dipole transitions in the intermediate coupling case, are higher in frequency than 350 GHz and are very weak. The strongest one of these is $J, K=2, 3-1, 0$ at 408643.9(4.0) MHz with a line strength of 0.042. For $^{33}\text{S}^{16}\text{O}$, the observed transitions are given in table 7. The relative intensities of the hyperfine transitions are included. Table 8 gives the observed rotational transitions of $^{32}\text{S}^{16}\text{O}$ in the first vibrational excited state and table 9, the spectral data of $^{32}\text{S}^{16}\text{O}$ in the electronic excited state $^1\Delta$. As a convenience to the user, the calculated transition frequencies from tables 4, 5, and 6 have been listed according to increasing frequency in table 10.

1.3. List of Symbols and Conversion Factors

a. Symbols

B_v	Rotational constant in the vibrational state v (MHz).
D_v	Quartic centrifugal distortion constant in the vibrational state v (MHz).
λ_v	Electron spin-spin coupling constant in the vibrational state v (MHz).
γ_v	Electron spin-rotation coupling constant in the vibrational state v (MHz).
ρ_v	Centrifugal distortion constant for λ_v (MHz).
$\lambda_{(1)}, \lambda_{(2)}$	First expansion parameters of λ in a power series of the internuclear distance; ρ_v is a combination of $\lambda_{(1)}$ and $\lambda_{(2)}$, but these param-

α_e	eters normally cannot be evaluated independently. If $\lambda_{(1)}$ is given, $\lambda_{(2)}$ is neglected in this work.	g_L^e	g -factor of the orbital angular momentum of electrons (Bohr magneton).
α_λ	First coefficient of the power series of B_v to $(v + \frac{1}{2})$: $B_v = B_e - \alpha_e(v + \frac{1}{2})$.	g_R	Rotational g -factor, including electronic and nuclear contributions. g_R is mostly denoted g_J in ${}^1\Sigma$ molecules (Bohr magneton).
B_e, λ_e	Extrapolated equilibrium values for B_v and λ_v , respectively.		
v	Vibrational state quantum number.		
J	Total angular momentum quantum number without nuclear spin.		
F	Total angular momentum quantum number including spin ($I=3/2$) of ${}^{33}\text{S}$.		
K	Rotational angular momentum quantum number; this is an approximate quantum number in the intermediate case between Hund's case a and b.		
eqQ	Nuclear electric quadrupole coupling constant of ${}^{33}\text{S}$ (MHz).		
b, c	Electron spin nuclear spin hyperfine coupling constants of ${}^{33}\text{S}$ (MHz).		
μ	Electric dipole moment (Debye).		
g_s^e	g -factor of the electron spin in SO (μ_B).		

b. Conversion Factors

The following conversion factors have been used:

$$B(\text{MHz}) = \frac{5.05376 \times 10^5}{I(\text{amu}\text{\AA}^2)} \quad (I = \text{moment of inertia})$$

$$1 \text{ cm}^{-1} \cong 29979.2456 \text{ MHz.}$$

The atomic masses used for the calculations in the isotopic relations were taken from A. H. Wapstra and N. B. Gove, Nuclear Data Tables **9**, 265 (1971).

1.4. References

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2. Sulfur Monoxide Spectral Tables

Table 1. Molecular Constants of Sulfur Monoxide

	${}^{32}\text{S}{}^{16}\text{O}$	${}^{34}\text{S}{}^{16}\text{O}$	${}^{32}\text{S}{}^{18}\text{O}$	Ref.
B_0 (MHz)	21523.5612 ± 0.010	21102.7219 ± 0.026	19929.1918 ± 0.066	73A
λ_0 (MHz)	158258.66 ± 2.4	158260.62 ± 9.8	158241.68 ± 30	73A
γ_0 (MHz)	-168.794 ± 0.30	-166.178 ± 1.14	-156.376 ± 4.0	73A
D_0 (MHz)	$(3.4207 \pm 0.018) \times 10^{-2}$ ^(a)	$(3.2877 \pm 0.018) \times 10^{-2}$ ^(a)	$(2.9318 \pm 0.018) \times 10^{-2}$ ^(b)	
ρ_0 (MHz)	0.2971 ± 0.10	0.2876 ± 0.030	0.2438 ± 0.070	73A
μ (Debye)	1.55 ± 0.02			64A
g_s^e	-2.00201 ± 0.00004	-2.00216 ± 0.00030		68B
g_L^e	$-(3.52 \pm 0.04) \times 10^{-3}$	$-(3.1 \pm 8) \times 10^{-3}$		68B
g_R	$-(1.2 \pm 0.4) \times 10^{-4}$	$-(6 \pm 5) \times 10^{-4}$		68B

^aRef. [68B].^bRef. [73A].Table 2. Molecular Constants of ${}^{33}\text{S}{}^{16}\text{O}$ in
the Ground Vibrational State.

B_0 (MHz)	21306.46 ± 0.10
λ_0 (MHz)	158257.3 ± 5.0

Table 2. Molecular Constants of $^{33}\text{S}^{16}\text{O}$ in
the Ground Vibrational State. (continued)

γ_0 (MHz)	-167.21±0.45
D_0 (MHz)	$(3.352\pm0.018)\times10^{-2}$
ρ_0 (MHz)	0.300±0.030
ϵQ (MHz)	-15.9±3.0 [67A]
b (MHz)	+51.0±2.0 [67A]
c (MHz)	-96.5±2.0 [67A]
μ (Debye)	1.55±0.05 [67A]

Table 3. Rotational Constants of $^{32}\text{S}^{16}\text{O}$ in the First
Excited Vibrational State and Equilibrium
Structure.

B_1 (MHz)	21351.61±0.20 [67A]
λ_1 (MHz)	159211.7±20 [67A]
γ_1 (MHz)	-171.26±2.0 [67A]
D_1 (MHz)	$(3.421\pm0.020)\times10^{-2}$
ρ_1 (MHz)	0.297±0.015
B_e (MHz)	21609.55±0.10
α_e (MHz)	171.96±0.20
λ_e (MHz)	157784±15
α_λ (MHz)	-952±23
r_e (\AA)	1.48108±0.00015

Table 4. Microwave Spectrum of $^{32}\text{S}^{16}\text{O}$ in the Ground Vibrational State (MHz).

Transition $J^{\prime}, K' - J'', K''$	Observed Frequency (Estimated Uncertainty) ^a	Calculated Frequency (Estimated Uncertainty) ^b	Line Strength	Upper State ^c	Lower State ^c	Ref.
1,0 - 0,1	30001.58(0.10)	30001.630(0.050)	[0.956]	1.001	0	67A
2,1 - 1,0	62931.80(0.20)	62931.731(0.046)	[1.936]	3.100	1.001	67A
1,1 - 1,0		286348.091(4.4)	[0.065]	10.552	1.001	
3,2 - 2,1	99299.87(0.10)	99299.875(0.062)	[2.933]	6.412	3.100	73A
2,2 - 1,1	86093.95(0.10)	86093.938(0.034)	[1.500]	13.424	10.552	73A
1,2 - 0,1		329393.458(4.4)	[0.044]	10.987	0	
2,2 - 2,1		309510.301(4.4)	[0.087]	13.424	3.100	
1,2 - 1,1	13043.70(0.10)	13043.745(0.042)	[1.435]	10.987	10.552	67A
1,2 - 2,1		236460.096(4.0)	[0.012]	10.987	3.100	
4,3 - 3,2	138178.60(0.50)	138178.548(0.098)	[3.938]	11.021	6.412	64B

Table 4. Microwave Spectrum of $^{32}\text{S}^{16}\text{O}$ in the Ground Vibrational State (MHz). (continued)

Transition $J',K' - J'',K''$	Observed Frequency (Estimated Uncertainty) ^a	Calculated Frequency (Estimated Uncertainty) ^b	Line Strength	Upper State ^c	Lower State ^c	Ref.
3,3 - 2,2	129138.85(0.10)	129138.862(0.053)	[2.667]	17.732	13.424	73A
2,3 - 1,2	109252.10(0.10)	109252.134(0.042)	[1.510]	14.632	10.987	73A
3,3 - 3,2		339349.287(4.4)	[0.095]	17.732	6.412	
2,3 - 2,2	36201.82(0.15)	36201.942(0.073)	[0.746]	14.632	13.424	73A
2,3 - 3,2		246412.359(4.3)	[0.012]	14.632	6.412	
5,4 - 4,3		178605.168(0.130)	[4.943]	16.979	11.021	
4,4 - 3,3	172181.46(0.50)	172181.316(0.068)	[3.750]	23.475	17.732	64B
3,4 - 2,3	158971.80(0.50)	158971.819(0.062)	[2.689]	19.934	14.632	64B
3,4 - 3,3	66034.94(0.20)	66034.890(0.075)	[0.488]	19.934	17.732	67A
3,4 - 4,3		267205.625(4.4)	[0.010]	19.934	11.021	
6,5 - 5,4		219949.093(0.166)	[5.948]	24.316	16.976	
5,5 - 4,4		215220.491(0.086)	[4.800]	30.654	23.475	
4,5 - 3,4		206176.043(0.111)	[3.781]	26.812	19.934	
4,5 - 4,4	100029.64(0.15)	100029.627(0.104)	[0.355]	26.812	23.475	73A
4,5 - 5,4		294776.511(4.6)	[0.007]	26.812	16.979	
7,6 - 6,5		261843.296(0.190)	[6.953]	33.050	24.316	
6,6 - 5,5		258255.555(0.103)	[5.833]	39.269	30.654	
5,6 - 4,5		251824.759(0.156)	[4.835]	35.212	26.812	
5,6 - 5,5		136634.896(0.21)	[0.275]	35.212	30.654	
5,6 - 6,5		326653.177(4.9)	[0.005]	35.212	24.316	
8,7 - 7,6		304077.299(0.21)	[7.957]	43.192	33.050	
7,7 - 6,6		301285.699(0.120)	[6.857]	49.318	39.269	
6,7 - 5,6		296549.966(0.192)	[5.870]	45.104	35.212	
6,7 - 6,6		174929.306(0.36)	[0.223]	45.104	39.269	
9,8 - 8,7		346527.791(0.22)	[8.960]	54.752	43.192	
8,8 - 7,7		344310.093(0.138)	[7.875]	60.803	49.318	
7,8 - 6,7		340714.034(0.22)	[6.894]	56.469	45.104	
7,8 - 7,7		214357.642(0.55)	[0.186]	56.469	49.318	
8,9 - 8,8		254574.351(0.76)	[0.159]	69.295	60.203	
9,10 - 9,9		295356.396(0.98)	[0.139]	83.575	73.723	
10,11 - 10,10		336554.652(1.22)	[0.123]	99.304	88.078	

^aError as it is given in the original reference.^cEnergy levels in cm⁻¹.^bError represents a 95% confidence level.Table 5. Microwave Spectrum of $^{34}\text{S}^{16}\text{O}$ in the Ground Vibrational State. Frequencies are in MHz units.

Transition $J',K' - J'',K''$	Observed Frequency (Estimated Uncertainty) ^a	Calculated Frequency (Estimated Uncertainty) ^b	Line Strength	Upper State ^c	Lower State ^c	Ref.
1,0 - 0,1	29678.98(0.10)	29679.089(0.16)	[0.958]	0.990	0	73A
2,1 - 1,0	62074.30(0.20)	62074.203(0.20)	[1.938]	3.061	0.990	67A
1,1 - 1,0		286677.128(18.)	[0.063]	10.552	0.990	
3,2 - 2,1	97715.39(0.15)	97715.340(0.32)	[2.935]	6.320	3.061	73A
2,2 - 1,1	84410.69(0.10)	84410.602(0.12)	[1.500]	13.368	10.552	73A
1,2 - 0,1		328880.885(18.)	[0.042]	10.970	0	
2,2 - 2,1		309013.528(18.)	[0.084]	13.368	3.061	
1,2 - 1,1	12524.30(0.20)	12524.668(0.14)	[1.437]	10.970	10.552	67A
1,2 - 2,1		237127.593(18.)	[0.012]	10.970	3.061	

Table 5. Microwave Spectrum of $^{34}\text{S}^{16}\text{O}$ in the Ground Vibrational State. Frequencies are in MHz units. (continued)

Transition $J',K' - J'',K''$	Observed Frequency (Estimated Uncertainty) ^a	Calculated Frequency (Estimated Uncertainty) ^b	Line Strength	Upper State ^c	Lower State ^c	Ref.
4,3 - 3,2		135775.330(0.50)	[3.939]	10.849	6.320	
3,3 - 2,2	126613.93(0.19)	126613.931(0.18)	[2.667]	17.591	13.368	73A
2,3 - 1,2	106742.92(0.15)	106743.123(0.16)	[1.509]	14.530	10.970	73A
3,3 - 3,2		337912.119(18.)	[0.093]	17.591	6.320	
2,3 - 2,2	34857.16(0.20)	34857.189(0.25)	[0.749]	14.530	13.368	67A
2,3 - 3,2		246155.376(18.)	[0.012]	14.530	6.320	
5,4 - 4,3		175352.198(0.69)	[4.944]	16.698	10.849	
4,4 - 3,3		168814.893(0.25)	[3.750]	23.222	17.591	
3,4 - 2,3		155506.704(0.25)	[2.688]	19.718	14.530	
3,4 - 3,3	63750.17(0.20)	63749.961(0.26)	[0.491]	19.718	17.591	67A
3,4 - 4,3		265886.750(19.)	[0.010]	19.718	10.849	
6,5 - 5,4		215839.149(0.84)	[5.949]	23.898	16.698	
5,5 - 4,4		211012.698(0.31)	[4.800]	30.260	23.222	
4,5 - 3,4		201846.696(0.42)	[3.780]	26.450	19.718	
4,5 - 4,4	96781.76(0.20)	96781.765(0.42)	[0.357]	26.450	23.222	73A
4,5 - 5,4		292381.248(20.)	[0.007]	26.450	16.698	
7,6 - 6,5		256876.837(0.95)	[6.953]	32.466	23.898	
6,6 - 5,5		253206.557(0.37)	[5.833]	38.707	30.260	
5,6 - 4,5		246663.500(0.60)	[4.834]	34.678	26.450	
5,6 - 5,5		132432.568(0.86)	[0.277]	34.678	30.260	
5,6 - 6,5		323205.600(21.)	[0.005]	34.678	28.898	
8,7 - 7,6		298256.785(1.05)	[7.957]	42.415	32.466	
7,7 - 6,6		295395.683(0.44)	[6.857]	48.560	38.707	
6,7 - 5,6		290562.209(0.70)	[5.870]	44.370	34.678	
6,7 - 6,6		169788.340(1.4)	[0.223]	44.370	38.707	
9,8 - 8,7		339855.845(1.1)	[8.960]	53.751	42.415	
8,8 - 7,7		337579.285(0.50)	[7.875]	59.821	48.560	
7,8 - 6,7		333900.953(0.84)	[6.894]	55.508	44.370	
7,8 - 1,1		208293.611(2.1)	[0.186]	55.508	40.560	
8,9 - 8,8		247600.596(2.9)	[0.159]	68.080	59.821	
9,10 - 9,9		287483.872(3.8)	[0.139]	82.077	72.488	
10,11 - 10,10		327792.281(4.7)	[0.123]	97.436	86.562	

^aError as it is given in the original reference.^bError represents a 95% confidence level.^cEnergy levels in cm⁻¹.Table 6. Microwave Spectrum of $^{32}\text{S}^{18}\text{O}$ in the Ground Vibrational State. Frequencies are in MHz units.

Transition $J',K' - J'',K''$	Observed Frequency (Estimated Uncertainty) ^a	Calculated Frequency (Estimated Uncertainty) ^b	Line Strength	Upper State ^c	Lower State ^c	Ref.
1,0 - 0,1		28722.845(0.20)	[0.963]	0.958	0	
2,1 - 1,0	59626.45(0.15)	59626.599(0.30)	[1.943]	2.947	0.958	73A
1,1 - 1,0		287605.115(25.)	[0.056]	10.552	0.958	
3,2 - 2,1	93267.27(0.20)	93267.198(0.45)	[2.939]	6.058	2.947	73A
2,2 - 1,1	79716.27(0.20)	79716.479(0.28)	[1.500]	13.211	10.552	73A
1,2 - 0,1		327462.027(25.)	[0.037]	10.923	0	
2,2 - 2,1		307694.995(25.)	[0.077]	13.211	2.947	

Table 6. Microwave Spectrum of $^{32}\text{S}^{18}\text{O}$ in the Ground Vibrational State. Frequencies are in MHz units. (continued)

Transition $J',K' - J'',K''$	Observed Frequency (Estimated Uncertainty) ^a	Calculated Frequency (Estimated Uncertainty) ^b	Line Strength	Upper State ^c	Lower State ^c	Ref.
1,2 - 1,1		11134.067(0.21)	[1.444]	10.923	10.557	
1,2 - 2,1		239112.583(25.)	[0.011]	10.923	2.947	
4,3 - 3,2		129065.750(0.55)	[3.941]	10.363	6.058	
3,3 - 2,2	+ 119572.79(0.40)	119572.959(0.36)	[2.667]	17.199	13.211	73A
2,3 - 1,2	99803.32(0.30)	99803.001(0.40)	[1.508]	14.252	10.923	73A
3,3 - 3,2		334000.756(25.)	[0.086]	17.199	6.058	
2,3 - 2,2		31220.589(0.31)	[0.757]	14.252	13.211	
2,3 - 3,2		245648.386(25.)	[0.012]	14.252	6.058	
5,4 - 4,3		166284.608(0.71)	[4.946]	15.910	10.363	
4,4 - 3,3		159427.329(0.42)	[3.750]	22.517	17.199	
3,4 - 2,3		145873.684(0.46)	[2.685]	19.118	14.252	
3,4 - 3,3		57521.314(0.37)	[0.498]	19.118	17.199	
3,4 - 4,3		262456.320(27.)	[0.010]	19.118	10.363	
6,5 - 5,4		204386.965(0.91)	[5.951]	22.728	15.910	
5,5 - 4,4		199278.884(0.59)	[4.800]	29.164	22.517	
4,5 - 3,4		189782.193(0.67)	[3.777]	25.448	19.118	
4,5 - 4,4		87876.178(0.66)	[0.362]	25.448	22.517	
4,5 - 5,4		285953.905(28.)	[0.007]	25.448	15.910	
7,6 - 6,5		243038.040(1.07)	[6.955]	30.834	22.728	
6,6 - 5,5		239126.921(0.74)	[5.833]	37.141	29.164	
5,6 - 4,5		232264.766(0.81)	[4.831]	33.196	25.448	
5,6 - 5,5		120862.060(1.04)	[0.282]	33.196	29.164	
5,6 - 6,5		313831.706(29.)	[0.005]	33.196	22.728	
8,7 - 7,6		282036.647(1.36)	[7.958]	40.242	30.834	
7,7 - 6,6		278970.735(0.83)	[6.857]	46.446	37.141	
6,7 - 5,6		273856.804(0.95)	[5.868]	42.331	33.196	
6,7 - 6,6		155591.943(1.80)	[0.226]	42.331	37.141	
9,8 - 8,7		321261.025(1.60)	[8.960]	50.958	40.242	
8,8 - 7,7		318809.626(1.04)	[7.875]	57.081	46.446	
7,8 - 6,7		314891.681(1.31)	[6.893]	52.834	42.331	
7,8 - 7,7		191512.889(2.5)	[0.188]	52.834	46.446	
8,9 - 8,8		228272.434(3.4)	[0.161]	64.695	57.081	
9,10 - 9,9		265639.189(4.6)	[0.140]	77.904	69.045	
10,11 - 10,10		303456.547(6.8)	[0.123]	92.457	82.335	

^aError as it is given in the original reference.^bError represents a 95% confidence level.^cEnergy levels in cm^{-1} .Table 7. Observed Microwave Transitions of $^{33}\text{S}^{16}\text{O}$ in the Ground Vibrational State. Frequencies are in MHz Units. Ref. [67A]

Transition $J',K' - J'',K''$	F' - F''	Observed Frequency (Estimated Uncertainty) ^b	Relative Intensity ^a
1,0 - 0,1	5/2 - 3/2	29857.30(0.50)	[0.500]
	3/2 - 3/2	29819.63(0.50)	[0.333]
	1/2 - 3/2	29805.98(0.50)	[0.167]
2,1 - 1,0	7/2 - 5/2	62506.20(0.50)	[0.400]
	5/2 - 3/2	62498.72(0.50)	[0.210]

Table 7. Observed Microwave Transitions of $^{33}\text{S}^{16}\text{O}$ in the Ground Vibrational State. Frequencies are in MHz Units. Ref. [67A]
(continued)

Transition $J',K' - J'',K''$	$F' - F''$	Observed Frequency (Estimated Uncertainty) ^b	Relative Intensity ^a
	3/2 - 1/2	62484.90(0.50)	[0.083]
	5/2 - 5/2	62461.10(0.50)	[0.090]
	3/2 - 3/2	62471.40(0.50)	[0.107]
	3/2 - 5/2	62433.68(0.50)	[0.010]
	1/2 - 3/2	62456.82(0.50)	[0.017]
1,2 - 1,1	5/2 - 5/2	12752.90(1.00)	[0.350]
	5/2 - 3/2	12695.08(0.50)	[0.150]
	3/2 - 5/2	12846.96(0.50)	[0.150]
	1/2 - 3/2	12839.40(0.50)	[0.139]
2,3 - 2,2	7/2 - 7/2	35469.40(0.50)	[0.343]
	5/2 - 5/2	35511.80(0.50)	[0.173]
	3/2 - 3/2	35541.20(0.50)	[0.080]
	3/2 - 5/2	35561.15(0.50)	[0.010]
3,4 - 3,3	9/2 - 9/2	64807.12(0.50)	[0.327]
	7/2 - 7/2	64853.15(0.50)	[0.218]
	5/2 - 5/2	64888.67(0.50)	[0.147]
	3/2 - 3/2	64914.21(0.50)	[0.114]

^aThe sum of the relative intensities of all hyperfine components for a specific transition $J',K' - J'',K''$ is 1.

^bError as given in the original reference; only the error on JK = 1,2 - 1,1 was increased by a factor of two due to an overlap with a line of $^{32}\text{S}^{16}\text{O}$, v = 1.

Table 8. Observed Microwave Transitions
of $^{32}\text{S}^{16}\text{O}$ in the First
Vibrational State. (MHz) Ref. [67A]

Transition $J',K' - J'',K''$	Observed Frequency (Estimated Uncertainty) ^a
1,0 - 0,1	29949.36(0.50)
2,1 - 1,0	62692.65(0.50)
1,2 - 1,1	12752.90(1.00)
2,3 - 2,2	35461.40(0.50)
3,4 - 3,3	64804.47(0.50)

^aError as given in the original reference; only the error on JK = 1,2 - 1,1 was increased by a factor of two due to an overlap with line of $^{33}\text{S}^{16}\text{O}$, v = 0.

Table 9. Spectral Data of $^{32}\text{S}^{16}\text{O}$ in the Electronic Excited State $1\Delta_2^*$ (MHz)

Transition	Observed Frequency (Estimated Uncertainty)	Ref.
$J' - J''$		
3 - 2	127770.47(0.15)	70A
B_0 (MHz)	21295.1±0.7	70A
μ (Debye)	1.336±0.045	70A
r_0 (Å)	1.49198±0.00010	70A

Table 10. Microwave Transitions of $^{32}\text{S}^{16}\text{O}$, $^{34}\text{S}^{16}\text{O}$, and $^{32}\text{S}^{18}\text{O}$ in Order of Frequency (unit MHz).

Calc. Frequency (MHz)	Molecule	Transition $J',K' - J'',K''$	Estimated Uncertainty ^a
11134.067	$^{32}\text{S}^{18}\text{O}$	1,2 - 1,1	(0.21)
12524.668	$^{34}\text{S}^{16}\text{O}$	1,2 - 1,1	(0.14)
13043.745	$^{32}\text{S}^{16}\text{O}$	1,2 - 1,1	(0.042)
28722.845	$^{32}\text{S}^{18}\text{O}$	1,0 - 0,1	(0.20)
29679.089	$^{34}\text{S}^{16}\text{O}$	1,0 - 0,1	(0.16)
30001.630	$^{32}\text{S}^{16}\text{O}$	1,0 - 0,1	(0.050)
31220.589	$^{32}\text{S}^{18}\text{O}$	2,3 - 2,2	(0.31)
34857.189	$^{34}\text{S}^{16}\text{O}$	2,3 - 2,2	(0.25)
36201.942	$^{32}\text{S}^{16}\text{O}$	2,3 - 2,2	(0.073)
57521.314	$^{32}\text{S}^{18}\text{O}$	3,4 - 3,3	(0.37)
59626.599	$^{32}\text{S}^{18}\text{O}$	2,1 - 1,0	(0.30)
62074.203	$^{34}\text{S}^{16}\text{O}$	2,1 - 1,0	(0.20)
62931.731	$^{32}\text{S}^{16}\text{O}$	2,1 - 1,0	(0.046)
63749.961	$^{34}\text{S}^{16}\text{O}$	3,4 - 3,3	(0.26)
66034.890	$^{32}\text{S}^{16}\text{O}$	3,4 - 3,3	(0.075)
79716.479	$^{32}\text{S}^{18}\text{O}$	2,2 - 1,1	(0.28)
84410.602	$^{34}\text{S}^{16}\text{O}$	2,2 - 1,1	(0.12)
86093.938	$^{32}\text{S}^{16}\text{O}$	2,2 - 1,1	(0.034)
87876.178	$^{32}\text{S}^{18}\text{O}$	4,5 - 4,4	(0.66)
93267.198	$^{32}\text{S}^{18}\text{O}$	3,2 - 2,1	(0.45)
96781.765	$^{34}\text{S}^{16}\text{O}$	4,5 - 4,4	(0.42)
97715.340	$^{34}\text{S}^{16}\text{O}$	3,2 - 2,1	(0.32)
99299.875	$^{32}\text{S}^{16}\text{O}$	3,2 - 2,1	(0.062)
99803.001	$^{32}\text{S}^{18}\text{O}$	2,3 - 1,2	(0.40)
100029.627	$^{32}\text{S}^{16}\text{O}$	4,5 - 4,4	(0.104)
106743.123	$^{34}\text{S}^{16}\text{O}$	2,3 - 1,2	(0.160)
109252.134	$^{32}\text{S}^{16}\text{O}$	2,3 - 1,2	(0.042)
119572.959	$^{32}\text{S}^{18}\text{O}$	3,3 - 2,2	(0.36)
120862.060	$^{32}\text{S}^{18}\text{O}$	5,6 - 5,5	(1.04)
126613.931	$^{34}\text{S}^{16}\text{O}$	3,3 - 2,2	(0.180)
129065.750	$^{32}\text{S}^{18}\text{O}$	4,3 - 3,2	(0.55)
129138.862	$^{32}\text{S}^{16}\text{O}$	3,3 - 2,2	(0.053)
132432.568	$^{34}\text{S}^{16}\text{O}$	5,6 - 5,5	(0.86)
135775.330	$^{34}\text{S}^{16}\text{O}$	4,3 - 3,2	(0.50)
136634.896	$^{32}\text{S}^{16}\text{O}$	5,6 - 5,5	(0.21)
138178.548	$^{32}\text{S}^{16}\text{O}$	4,3 - 3,2	(0.098)
145873.684	$^{32}\text{S}^{18}\text{O}$	3,4 - 2,3	(0.46)
155506.704	$^{34}\text{S}^{16}\text{O}$	3,4 - 2,3	(0.25)
155591.943	$^{32}\text{S}^{16}\text{O}$	6,7 - 6,6	(1.80)

Table 10. Microwave Transitions of $^{32}\text{S}^{16}\text{O}$, $^{34}\text{S}^{16}\text{O}$ and $^{32}\text{S}^{18}\text{O}$ in Order of Frequency (unit MHz). (continued)

Calc. Frequency (MHz)	Molecule	Transition $J',K' - J'',K''$	Estimated Uncertainty ^a
158971.819	$^{32}\text{S}^{16}\text{O}$	3,4 - 2,3	(0.062)
159427.329	$^{32}\text{S}^{18}\text{O}$	4,4 - 3,3	(0.42)
166284.608	$^{32}\text{S}^{18}\text{O}$	5,4 - 4,3	(0.71)
168814.893	$^{34}\text{S}^{16}\text{O}$	4,4 - 3,3	(0.25)
169788.340	$^{34}\text{S}^{16}\text{O}$	6,7 - 6,6	(1.40)
172181.316	$^{32}\text{S}^{16}\text{O}$	4,4 - 3,3	(0.068)
174929.306	$^{32}\text{S}^{16}\text{O}$	6,7 - 6,6	(0.36)
175352.198	$^{34}\text{S}^{16}\text{O}$	5,4 - 4,3	(0.69)
178605.168	$^{32}\text{S}^{16}\text{O}$	5,4 - 4,3	(0.130)
189782.193	$^{32}\text{S}^{18}\text{O}$	4,5 - 3,4	(0.67)
191512.889	$^{32}\text{S}^{18}\text{O}$	7,8 - 7,7	(2.5)
199278.884	$^{32}\text{S}^{18}\text{O}$	5,5 - 4,4	(0.59)
201846.696	$^{34}\text{S}^{16}\text{O}$	4,5 - 3,4	(0.42)
204386.965	$^{32}\text{S}^{18}\text{O}$	6,5 - 5,4	(0.91)
206176.043	$^{32}\text{S}^{16}\text{O}$	4,5 - 3,4	(0.111)
208293.611	$^{34}\text{S}^{16}\text{O}$	7,8 - 7,7	(2.1)
211012.698	$^{34}\text{S}^{16}\text{O}$	5,5 - 4,4	(0.31)
214357.642	$^{32}\text{S}^{16}\text{O}$	7,8 - 7,7	(0.55)
215220.491	$^{32}\text{S}^{16}\text{O}$	5,5 - 4,4	(0.086)
215839.149	$^{34}\text{S}^{16}\text{O}$	6,5 - 5,4	(0.84)
219949.093	$^{32}\text{S}^{16}\text{O}$	6,5 - 5,4	(0.166)
228272.434	$^{32}\text{S}^{18}\text{O}$	8,9 - 8,8	(3.4)
232264.766	$^{32}\text{S}^{18}\text{O}$	5,6 - 4,5	(0.81)
236460.096	$^{32}\text{S}^{16}\text{O}$	1,2 - 2,1	(4.0)
237127.593	$^{34}\text{S}^{16}\text{O}$	1,2 - 2,1	(18.)
239112.583	$^{32}\text{S}^{18}\text{O}$	1,2 - 2,1	(25.)
239126.921	$^{32}\text{S}^{18}\text{O}$	6,6 - 5,5	(0.74)
243038.040	$^{32}\text{S}^{18}\text{O}$	7,6 - 6,5	(1.07)
243648.386	$^{32}\text{S}^{18}\text{O}$	2,3 - 2,2	(25.)
246155.376	$^{34}\text{S}^{16}\text{O}$	2,3 - 3,2	(18.)
246412.359	$^{32}\text{S}^{16}\text{O}$	2,3 - 3,2	(4.3)
246663.500	$^{34}\text{S}^{16}\text{O}$	5,6 - 4,5	(0.60)
247600.596	$^{34}\text{S}^{16}\text{O}$	8,9 - 8,8	(2.9)
251824.759	$^{32}\text{S}^{16}\text{O}$	5,6 - 4,5	(0.156)
251206.557	$^{34}\text{S}^{16}\text{O}$	6,6 - 5,5	(0.37)
254574.351	$^{32}\text{S}^{16}\text{O}$	8,9 - 8,8	(0.76)
256876.897	$^{34}\text{S}^{16}\text{O}$	7,6 - 6,5	(0.95)
258255.555	$^{32}\text{S}^{16}\text{O}$	6,6 - 5,5	(0.103)
261843.296	$^{32}\text{S}^{16}\text{O}$	7,6 - 6,5	(0.190)
262456.320	$^{32}\text{S}^{18}\text{O}$	3,4 - 4,3	(27.)
265639.189	$^{32}\text{S}^{18}\text{O}$	9,10 - 9,9	(4.6)
265886.750	$^{34}\text{S}^{16}\text{O}$	3,4 - 4,3	(19.)
267205.625	$^{32}\text{S}^{16}\text{O}$	3,4 - 4,3	(4.4)
273856.804	$^{32}\text{S}^{18}\text{O}$	6,7 - 5,6	(0.95)
278970.735	$^{32}\text{S}^{18}\text{O}$	7,7 - 6,6	(0.83)
282036.647	$^{32}\text{S}^{18}\text{O}$	8,7 - 7,6	(1.36)
285953.905	$^{32}\text{S}^{18}\text{O}$	4,5 - 5,4	(28.)
286348.091	$^{32}\text{S}^{16}\text{O}$	1,1 - 1,0	(4.4)
286677.128	$^{34}\text{S}^{16}\text{O}$	1,1 - 1,0	(18.)
287483.872	$^{34}\text{S}^{16}\text{O}$	9,10 - 9,9	(3.8)
287605.115	$^{32}\text{S}^{18}\text{O}$	1,1 - 1,0	(25.)

Table 10. Microwave Transitions of $^{32}\text{S}^{16}\text{O}$, $^{34}\text{S}^{16}\text{O}$ and $^{32}\text{S}^{18}\text{O}$
in Order of Frequency (unit MHz). (continued)

Calc. Frequency (MHz)	Molecule	Transition $J^{\prime}, K^{\prime} - J^{\prime\prime}, K^{\prime\prime}$	Estimated Uncertainty ^a
290562.209	$^{34}\text{S}^{16}\text{O}$	6,7 - 5,6	(0.70)
292381.248	$^{34}\text{S}^{16}\text{O}$	4,5 - 5,4	(20.)
294776.511	$^{32}\text{S}^{16}\text{O}$	4,5 - 5,4	(4.6)
295356.396	$^{32}\text{S}^{16}\text{O}$	9,10 - 9,9	(0.98)
295395.683	$^{34}\text{S}^{16}\text{O}$	7,7 - 6,6	(0.44)
296549.966	$^{32}\text{S}^{16}\text{O}$	6,7 - 5,6	(0.192)
298256.785	$^{34}\text{S}^{16}\text{O}$	8,7 - 7,6	(1.05)
301285.699	$^{32}\text{S}^{16}\text{O}$	7,7 - 6,6	(0.120)
303456.547	$^{32}\text{S}^{18}\text{O}$	10,11 - 10,10	(6.8)
304077.299	$^{32}\text{S}^{16}\text{O}$	8,7 - 7,6	(0.21)
307694.995	$^{32}\text{S}^{18}\text{O}$	2,2 - 2,1	(25.)
309013.528	$^{34}\text{S}^{16}\text{O}$	2,2 - 2,1	(18.)
309510.301	$^{32}\text{S}^{16}\text{O}$	2,2 - 2,1	(4.4)
313831.706	$^{32}\text{S}^{18}\text{O}$	5,6 - 6,5	(29.)
314891.681	$^{32}\text{S}^{18}\text{O}$	7,8 - 6,7	(1.31)
318809.626	$^{32}\text{S}^{18}\text{O}$	8,8 - 7,7	(1.04)
321261.025	$^{32}\text{S}^{18}\text{O}$	9,8 - 8,7	(1.60)
323205.600	$^{34}\text{S}^{16}\text{O}$	5,6 - 6,5	(21.)
326653.177	$^{32}\text{S}^{16}\text{O}$	5,6 - 6,5	(4.9)
327462.027	$^{32}\text{S}^{18}\text{O}$	1,2 - 0,1	(25.)
327792.281	$^{34}\text{S}^{16}\text{O}$	10,11 - 10,10	(4.7)
328880.885	$^{34}\text{S}^{16}\text{O}$	1,2 - 0,1	(18.)
329393.458	$^{32}\text{S}^{16}\text{O}$	1,2 - 0,1	(4.4)
333900.953	$^{34}\text{S}^{16}\text{O}$	7,6 - 6,7	(0.84)
334000.756	$^{32}\text{S}^{18}\text{O}$	3,3 - 3,2	(25.)
336554.652	$^{32}\text{S}^{16}\text{O}$	10,11 - 10,10	(1.22)
337579.285	$^{34}\text{S}^{16}\text{O}$	8,8 - 7,7	(0.50)
337912.119	$^{34}\text{S}^{16}\text{O}$	3,3 - 3,2	(18.)
339349.287	$^{32}\text{S}^{16}\text{O}$	3,3 - 3,2	(4.4)
339855.845	$^{34}\text{S}^{16}\text{O}$	9,8 - 8,7	(1.10)
340714.034	$^{32}\text{S}^{16}\text{O}$	7,8 - 6,7	(0.22)
344310.093	$^{32}\text{S}^{16}\text{O}$	8,8 - 7,7	(0.138)
346527.791	$^{32}\text{S}^{16}\text{O}$	9,8 - 8,7	(0.22)

^aError represents a 95% confidence level.

2.1. Laboratory References on Sulfur Monoxide

a. Microwave Spectrum

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b. Electron Paramagnetic Resonance

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2.2 Interstellar References on Sulfur Monoxide

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