

# Microwave Spectra of Molecules of Astrophysical Interest

## VI. Carbonyl Sulfide and Hydrogen Cyanide

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All available data on the microwave spectra of carbonyl sulfide and hydrogen cyanide are critically reviewed and tabulated. Molecular data such as rotational constants, centrifugal distortion constants, dipole moments, hyperfine coupling constants, and structural parameters are also tabulated. All rotational transitions from 100 MHz to 300 GHz that are deemed likely to be of interest to radio astronomers are calculated and tabulated along with their estimated 95 percent confidence limits. Microwave measurements are tabulated for most isotopic species and for many of the lower vibrational states. For both carbonyl sulfide and hydrogen cyanide a bibliography is given which includes nearly all the spectroscopic work reported in the literature. For each molecule a bibliography of related astrophysical papers is also given.

**Keywords:** Carbonyl sulfide; hydrogen cyanide; interstellar molecules; microwave spectra; molecular parameters; radio astronomy; rotational transitions; spectra.

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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 in interstellar observations. Although this review is designed to fulfill the needs of radio astronomers, it is expected that other workers may find such a review useful; consequently an effort has been made to include all microwave measurements made on all isotopes of OCS and HCN. No attempt has been made to include all types of spectral or structural measurements which have been made on these molecules although the references do include many papers on line width measurements and infrared measurements as well as microwave measurements.

Radio astronomers will be primarily interested in tables 5, 6, and 7 for OCS and table 16 for HCN. This review covers all the information available as of July 1, 1973.

In using these tables the reader is cautioned to remember that all observed transitions are tabulated even though the observations are in some cases outdated and consequently less accurate than the calculated transition frequencies. Every effort has been made to fairly evaluate the error limits or uncertainties assigned to the listed observations even though the original publications were often remiss in providing that information. In some cases where uncertainties were given in the original publication we have taken the liberty of using a different uncertainty based on more recent work.

Wherever possible the data were combined in a least squares analysis in which each measurement was weighted by the inverse square of its estimated uncertainty. In only a few cases were sufficient data available to form a statistical basis for estimating the reliability of the rotational constants and of transitions calculated from those constants. In all other cases the uncertainties were estimated in a more subjective fashion from the uncertainties given for the measurements and from considerations such as the model error caused by the omission of higher order terms. The uncertainties quoted in the tables are equivalent to a 95 percent confidence level (about two standard deviations).

The molecular constants given in the tables are quoted with enough significant figures to allow one to reproduce the original fit to the observed transitions without reduction in accuracy due to round-off. This is done for the sake of consistency even though the estimated standard deviations may indicate that the constants are known with much less accuracy.

A full description of the theory of rotational spectra (including equations relating the rotational constants to the measured transitions) is given in a number of texts which discuss microwave spectroscopy, but the books by Townes and Schawlow [1],<sup>1</sup> and Gordy

and Cook [2] are particularly thorough and use notation which is consistent with that used in these tables. One exception is the description of *l*-type resonance (not to be confused with *l*-type doubling) which is not covered in most texts but is described in ref. 3 in conjunction with the measurements on HCN and DCN given in tables 22 and 23.

Many of the tables give rotational constants or transition frequencies for different vibrational states. According to the convention set forth in ref. 4, the notation that should be used for asymmetric linear triatomic molecules is as follows:  $\nu_1$  represents the higher frequency stretching vibration,  $\nu_2$  represents the bending vibration, and  $\nu_3$  represents the lower frequency stretching vibration. This notation is used throughout these tables even though the primary reference sources have not followed the above convention, but have reversed the meaning of  $\nu_1$  and  $\nu_3$ .

In general these tables avoid the use of calculated constants or transitions except where they are a direct result of experimental measurements. A notable exception is the tabulation of rotational constants (tables 1, 3, 4, 13, and 15) where it was necessary to correct for the effect of centrifugal distortion even when the observed transitions did not provide a measure of the distortion constant. In the case of HCN the observed centrifugal distortion was in perfect agreement with that calculated in ref. 5. Consequently, the missing centrifugal distortion constants for HCN were taken from ref. 5 in order to determine the appropriate *B* values for tables 13 and 15 and to calculate some of the transitions given in table 16. For OCS the missing distortion constants were estimated by interpolation or extrapolation from the measured values for other species.

Unlike other papers in this series, the present tables do not tabulate line strengths other than the relative intensities of the quadrupole hyperfine components of resolved transitions. This is because the line strength (*S*) is a simple function of the quantum numbers as follows:

for  $\Delta J = +1$

$$S(J', J'') = \frac{(J')^2 - l^2}{J'},$$

while for  $\Delta J = 0$

$$S(J, J) = \frac{(2J+1) l^2}{J(J+1)}.$$

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

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

where  $\nu$  is the transition frequency in MHz and  $\mu$  is the dipole moment in Debyes.

<sup>1</sup>Figures in brackets indicate literature references.

## 1.1. List of Symbols and Conversion Factors

## a. Symbols

$B$	Rotational constant (MHz). ( $B = \frac{\hbar}{8\pi^2 I}$ ).
$I$	Moment of inertia of the molecule.
$D$	Quartic centrifugal distortion constant.
$H$	Sextic centrifugal distortion constant.
$q$	$l$ -doubling constant.
$J$	Total rotational angular momentum quantum number.
$F_x$	Angular momentum quantum number which includes the rotational angular momentum and the nuclear spin for the nucleus with largest $eqQ$ (nucleus x).
$F$	Total angular momentum quantum number including the spin of all nuclei.
$(eqQ)_x$	Nuclear electric quadrupole coupling constant related to nucleus x.
$eqQ\eta$	Product of the nuclear quadrupole coupling constant and the asymmetry parameter for the bending vibrational state.
$r_c(X - Y)$	Equilibrium distance between centers of mass of atoms X and Y (Å).
$\mu$	Dipole moment of the molecule (Debye units).
$l$	Quantum number for vibrational angular momentum.
$v_i$	Quantum number for the $i$ 'th vibrational state.
$\sigma_{  }, \sigma_{\perp}$	Components of the magnetic shielding tensor which are parallel and perpendicular to the molecular axis, respectively.
$\theta$	Molecular quadrupole moment relative to the center of mass.
$\alpha_{  } - \alpha_{\perp}$	Electric polarizability anisotropy.
$\chi_{\perp}, \chi_{  }$	Components of the magnetic susceptibility tensor which are respectively perpendicular and parallel to the molecular axis.
$\chi_{xx} - \chi_{yy}$	Magnetic susceptibility anisotropy.
$g_{\perp}, g_{  }$	Components of the molecular $\mathbf{G}$ tensor which are respectively perpendicular and parallel to the molecular axis. $g_{\perp}$ is sometimes denoted $g$ or $g_J$ for linear molecules in the ground state.
$g_{xx} - g_{yy}$	Anisotropy of the molecular $\mathbf{G}$ tensor perpendicular to the molecular axis.
$C_x$	Spin rotation constant related to nucleus x.
$S_{xy}$	Spin-spin interaction constant between nucleus x and nucleus y.
(. . .)	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.

## b. Conversion Factors

The following conversion factors have been used:

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

$$1 \text{ cm}^{-1} = 29,979.2456 \text{ MHz}^2$$

## 1.2. References

- [1] C. H. Townes and A. L. Schawlow, *Microwave Spectroscopy*, McGraw-Hill, New York, 1955.
- [2] W. Gordy and R. L. Cook, *Microwave Molecular Spectra*, John Wiley & Sons, New York, 1970.
- [3] A. G. Maki and D. R. Lide, *J. Chem. Phys.* **47**, 3206 (1967). "Microwave and Infrared Measurements on HCN and DCN: Observations on  $l$ -Type Reasonance Doublets."
- [4] R. S. Mulliken, *J. Chem. Phys.* **23**, 1997 (1955). "Report on Notation for the Spectra of Polyatomic Molecules."
- [5] T. Nakagawa and Y. Morino, *J. Mol. Spectrosc.* **31**, 208 (1969). "Higher-Order Variations of  $l$ -Type Doubling Constants and Centrifugal Distortion Constants for HCN and OCS."

## 2. Carbonyl Sulfide

## 2.1. Organization of the Spectral Tables

Tables 5, 6, and 7 contain both observed and calculated rotational transitions for the four most abundant isotopic species of carbonyl sulfide in the ground vibrational state. These tables also give the energy in  $\text{cm}^{-1}$  of both the upper and lower states involved in each transition. These tables were arbitrarily cut off at a frequency of 300 GHz although higher observed transitions were included in table 5. Since the  $\Delta J = 0$   $l$ -doublet transitions given in tables 11 and 12 are extremely weak at or below room temperature, they include only the range of transitions observed in the laboratory. Tables 8, 9, and 10 also include only those transitions observed in the laboratory. Should one wish to predict other transitions, they can be calculated by using the constants given in tables 1, 3, or 4.

For those molecules which contain  $^{17}\text{O}$ ,  $^{35}\text{S}$ , or  $^{33}\text{S}$ , tables 8 and 10 give observed transitions due to the different quadrupole components. In table 8 the calculated quadrupole splittings and relative intensities are also given. The calculated unsplit frequencies are given opposite the  $J$  quantum numbers.

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

## 2.2. Carbonyl Sulfide Spectral Tables

Table 1. Molecular constants for carbonyl sulfide

Molecule	$B_0$ (MHz)	$D_0$ (kHz)	$\epsilon_{eq}Q$ (MHz)
$^{16}_0{}^{12}C{}^{32}S^a$	6081.492439(134)	1.301789(150)	----
$^{16}_0{}^{12}C{}^{34}S$	5932.8379(50)	1.2691(370)	----
$^{16}_0{}^{13}C{}^{32}S$	6061.92498(84)	1.29898(225)	----
$^{18}_0{}^{12}C{}^{32}S$	5704.8607(4)[73A]	1.1353(160)[73A]	----
$^{16}_0{}^{13}C{}^{34}S$	5911.733(4) [73A]	----	----
$^{18}_0{}^{12}C{}^{34}S$	5559.971(5) [73A]	----	----
$^{18}_0{}^{13}C{}^{32}S$	5691.069(5) [73A]	----	----
$^{18}_0{}^{13}C{}^{34}S$	5544.864(20)[73A]	----	----
$^{16}_0{}^{14}C{}^{32}S$	6043.26(50) [48A]	----	----
$^{17}_0{}^{12}C{}^{32}S$	5883.675(20)[73B]	----	-1.32(14) [52B]
$^{16}_0{}^{12}C{}^{33}S$	6004.922(6) [51A]	----	-29.1184(12)[73C]
$^{16}_0{}^{12}C{}^{35}S$	5864.371(7) [51A]	----	21.90(8) [54B]
$^{16}_0{}^{12}C{}^{36}S$	5799.680(25)[49B]	----	----

Structure

linear

$$r_e \text{ (C-S)} \quad 1.5628 \pm 0.0010 \text{ \AA} \quad [73A]$$

$$r_e \text{ (O-C)} \quad 1.1543 \pm 0.0010 \text{ \AA} \quad [73A]$$

<sup>a</sup>For  $^{16}_0{}^{12}C{}^{32}S$   $H_0 \approx -2 \pm 2 \times 10^{-5}$  Hz.

Table 2. Hyperfine constants and dipole moment for carbonyl sulfide

	$^{16}_O^{12}C^{32}S$	$^{16}_O^{12}C^{34}S$	$^{16}_O^{13}C^{32}S$	$^{18}_O^{12}C^{32}S$	$^{16}_O^{12}C^{33}S$
$\mu(v_2=0)$ (Debyes) <sup>a,b</sup>	0.71519(3) [73C]	----	----	----	----
$\mu(v_2=1)$ (Debyes) <sup>a,b</sup>	0.70433(3) [73C]	----	----	----	----
$\mu(v_2=1)/\mu(v_2=0)$	0.98482(2) [73C]	----	----	----	----
$\mu(v_2=0)/\mu(^{16}_O^{12}C^{32}S, v_2=0)$	1.00000	1.00031(2) [73C]	1.00017(2) [73C]	0.99904(3) [73C]	1.00024(25) [73C]
$\mu(v_2=1)/\mu(^{16}_O^{12}C^{32}S, v_2=1)$	1.00000	1.00033(2) [73C]	1.00067(2) [73C]	0.99907(4) [73C]	1.00012(9) [73C]
$\sigma_{  } - \sigma_{\perp}$ ( $\text{cm}^3$ )	$4.67(16) \times 10^{-24}$ [70A]	----	----	----	----
$\theta$ ( $\text{esu} \cdot \text{cm}^2$ )	$-0.786(14) \times 10^{-26}$ [70C]	$-0.858(23) \times 10^{-26}$ [70C]	$-0.716(40) \times 10^{-26}$ [70C]	----	----
$x_{\perp} - x_{  }$ ( $\text{kHz}/\text{kG}^2$ )	2.348(3) [70C]	2.342(5) [70C]	2.360(9) [70C]	----	----
$x_{\perp} - x_{  }$ ( $v_2=1$ ) ( $\text{kHz}/\text{kG}^2$ )	2.38(10) [72B]	----	----	----	----
$x_{xx} - x_{yy}$ ( $v_2=1$ ) ( $\text{kHz}/\text{kG}^2$ )	-0.03(3) [72B]	----	----	----	----
$g_{\perp}(v_2=0)$	-0.028839(6) [70C]	-0.028242(10) [70C]	-0.028710(15) [70C]	----	----
$g_{\perp}(v_2=1)$	-0.02930(4) [72B]	----	----	----	----
$g_{  } - g_{\perp}(v_2=1)$	0.0905(5) [72B]	----	----	----	----
$g_{xx} - g_{yy}(v_2=1)$	0.00023(2) [72B]	----	----	----	----
$C_{13}C$ (kHz)	----	----	3.1(2) [70C]	----	----
$\sigma_{  } - \sigma_{\perp}$	----	----	$372(42) \times 10^{-6}$ [70C]	----	----

<sup>a</sup>Determined from data used for ref. 70C and 72B but revised to correspond with  $\hbar = 6.626196(50) \times 10^{-34} \text{ J s}$ .<sup>b</sup>Polarity determined to be  ${}^+OCS$  [69A].

Table 3. Rotational constants for the lower vibrational states of the most abundant isotopic species of OCS

Vib. State <sup>a</sup> $v_1^f$ $v_2$ $v_3$	$^{16}_0\text{C}^{32}\text{S}$ [ref. 6A]			$^{16}_0\text{C}^{32}\text{S}$ [ref. 7A]			$^{16}_0\text{C}^{32}\text{S}$ [ref. 73A]			$^{18}_0\text{C}^{32}\text{S}$ [ref. 73A]		
	$B_v$ (MHz)	$D_v$ (kHz)	$q_v$ (MHz)	$B_v$ (MHz)	$q_v$ (MHz)	$D_v$ (kHz)	$B_v$ (MHz)	$q_v$ (MHz)	$D_v$ (kHz)	$B_v$ (MHz)	$q_v$ (MHz)	
0 1 0	6092.07822(46) <sup>b</sup>	1.32359(90) <sup>b</sup>		6.36141271(161) <sup>c</sup>	5943.158(10)	6.0698022(100) <sup>d</sup>	6071.913(4)	6.5078448(52) <sup>e</sup>	5714.995(4)	1.198(15)	5.653026(10) <sup>f</sup>	0 1 <sup>1</sup> 0
				$\times 10^{-6}$ J(J+1)		$\times 10^{-6}$ J(J+1)		$\times 10^{-6}$ J(J+1)		$\times 10^{-6}$ J(J+1)	$\times 10^{-6}$ J(J+1)	
0 2 0	6100.19116(131) <sup>b</sup>	1.0966(35) <sup>b</sup>		5951.273(10)		6079.250(5)	1.133(38)	5722.924(5)	1.020(33)		0 2 0	
0 2 0	6102.55931(76) <sup>b</sup>	1.34174(260) <sup>b</sup>		5953.392(10)		6081.801(7)	1.363(46) <sup>g</sup>	5725.024(4)	1.156(20) <sup>g</sup>		0 2 0	
0 3 0	6108.626(12)		6.183(20)			6087.031(5)	6.287(5)	5731.142(7)		5.504(7)	0 3 0	
0 3 0	6112.925(12)				6091.583(5)			5734.973(5)	1.304(24)		0 3 0	
0 4 0	6114.723(20)				6092.200(17)			5737.002(10)		0 4 0		
0 4 0	6117.310(20)				6095.070(8)			5739.504(10)		0 4 0		
0 4 0	6123.244(20)				6101.262(9)			5744.819(10)	1.284(71)		0 4 0	
0 5 0	6121.724(30)			6.055(30)						0 5 0		
0 0 1	6063.35744(104) <sup>b</sup>	1.32734(278) <sup>b</sup>		5915.152(10)		6043.949(5)	1.403(35)	5688.653(5)	1.170(25)		0 0 1	
0 1 1	6075.503(15)			6.856(20)		6055.610(8)		5700.182(6)		6.053(11)	0 1 1	
0 2 1	6084.385(20)					6063.680(13)		5708.826(12)		0 2 1		
0 2 1	6087.227(20)					6066.811(17)		5711.369(17)	1.386(81) <sup>h</sup>		0 2 1	
0 3 1	6093.56(10)			6.50(10)						0 3 1		
0 3 2	6044.873(20)					5897.120(20)		5672.140(10)		0 0 2		
0 1 2	6058.536(30)			7.285(20)				6025.643(12)		0 1 2		
1 0 0	5045.051(20)					5897.390(20)		6027.649(19)		1 0 0		
1 1 0	6056.259(30)			6.450(20)						1 1 0		

<sup>a</sup>Note that these tables use a different vibrational numbering from that used in the primary references (see explanation in the Introduction).<sup>b</sup>Ref. 74A.<sup>c</sup>Ref. 72B and 67C.<sup>d</sup>Ref. 73C.<sup>e</sup>Ref. 67C and 73C.<sup>f</sup>Ref. 73A and 73C.<sup>g</sup> $D(02^{2c}0) = 1.57422(260)$  kHz for  $^{16}_0\text{C}^{32}\text{S}$ , 1.597(66) kHz for  $^{16}_0\text{C}^{32}\text{S}$ , and 1.335(20) kHz for  $^{18}_0\text{C}^{32}\text{S}$ ; the values given in this table are  $D(02^{2d}0)$ .<sup>h</sup>Average value for both c and d components.

Table 4. Molecular constants for vibrational states of less abundant isotopic species of carbonyl sulfide (Ref. 73A)

Molecule	Vibrational <sup>a</sup> State $v_1$ $v_2$ $v_3$			$E_v$ (MHz)	$g_v$ (MHz)
$^{16}_0\text{C}^{34}\text{S}$	0	$1^1$	0	$5921.462 \pm 0.015$	$6.199 \pm 0.015$
	0	$2^0$	0	$5928.866 \pm 0.010$	-
	0	$2^2$	0	$5911.050 \pm 0.010$	-
	0	$0^0$	1	$5894.148 \pm 0.010$	-
$^{18}_0\text{C}^{34}\text{S}$	0	$1^1$	0	$5569.845 \pm 0.013$	$5.393 \pm 0.013$
	0	$2^0$	0	$5577.726 \pm 0.015$	-
	0	$0^0$	1	$5544.199 \pm 0.010$	-
$^{18}_0\text{C}^{32}\text{S}$	0	$1^1$	0	$5700.627 \pm 0.020$	$5.800 \pm 0.020$
	0	$0^0$	1	$5674.994 \pm 0.040$	-
$^{16}_0\text{C}^{32}\text{S}$	0	$1^1$	0	$6052.65 \pm 0.80^b$	$6.70 \pm 0.20^b$
$^{16}_0\text{C}^{33}\text{S}$	0	$1^1$	0	$6015.47 \pm 0.20^c$	$6.21 \pm 0.20^c$
	0	$2^0$	0	$6023.11 \pm 0.25^c$	-
	0	$0^0$	1	$5986.86 \pm 0.25^c$	-

<sup>a</sup>Note that these tables use a different vibrational numbering from that used in the primary references (see explanation in the Introduction).

<sup>b</sup>From Ref. 48A.

<sup>c</sup>From Ref. 68B.

Table 5. Microwave Spectrum of  $^{16}_0\text{C}^{32}\text{S}$  in the Ground Vibrational State.

Transition $J^{\prime}-J''$	Obs. Freq. in MHz (Est. Unc.)	Cal. Freq. in MHz (Est. Unc.)	Energy in $\text{cm}^{-1}$		Ref.
			Upper State	Lower State	
1- 0	12 162.972(30)	12 162.9797(3)	0.406	0.0	67B
2- 1	24 325.930(20)	24 325.9281(5)	1.217	0.406	74A
3- 2	36 488.8128(20)	36 488.8140(8)	2.434	1.217	69B
4- 3	48 651.64(30)	48 651.6063(11)	4.057	2.434	49A
5- 4	60 814.270(20)	60 814.2735(13)	6.086	4.057	74A
6- 5	72 976.796(20)	72 976.7845(15)	8.520	6.086	74A
7- 6	85 139.106(10)	85 139.1081(18)	11.360	8.520	72C, 74A
8- 7	97 301.212(20)	97 301.2130(20)	14.605	11.360	74A
9- 8	109 463.063(10)	109 463.0679(21)	18.257	14.605	70B
10- 9	121 624.638(10)	121 624.6416(23)	22.314	18.257	70B
11-10	133 785.900(10)	133 785.9029(25)	26.776	22.314	70B
12-11	145 946.821(10)	145 946.8205(26)	31.645	26.776	70B
13-12	158 107.360(10)	158 107.3632(28)	36.918	31.645	70B
14-13	170 267.494(10)	170 267.4998(29)	42.598	36.918	70B
15-14	182 427.198(10)	182 427.1989(30)	48.683	42.598	70B
16-15	194 586.433(10)	194 586.4294(32)	55.174	48.683	70B
17-16	206 745.161(10)	206 745.1600(33)	62.070	55.174	70B
18-17	218 903.374(30)	218 903.3594(35)	69.372	62.070	74A
19-18	231 061.022(30)	231 060.9965(37)	77.079	69.372	74A
20-19	243 218.040(10)	243 218.0399(39)	85.192	77.079	70B
21-20	255 374.461(10)	255 374.458(4)	93.711	85.192	70B
22-21	267 530.239(30)	267 530.221(5)	102.634	93.711	74A
23-22	279 685.318(30)	279 685.296(5)	111.964	102.634	74A
24-23	291 839.686(30)	291 839.652(5)	121.698	111.964	74A
25-24	303 993.242(20)	303 993.259(6)	131.839	121.698	74A
26-25	316 144.7(20)	316 146.084(6)	142.384	131.839	54C
28-27	340 449.2(20)	340 449.267(8)	164.691	153.335	54C
30-29	364 747.5(30)	364 748.950(9)	188.619	176.453	54C
32-31	389 041. (4)	389 044.883(11)	214.168	201.191	54C
40-39	486 184.2(30)	486 186.123(19)	332.568	316.351	56A
42-41	510 457.3(30)	510 459.559(20)	366.218	349.191	56A
58-57	704 437.052(30)	704 437.056(21)	693.667	670.170	70D
59-58	716 546.559(30)	716 546.571(21)	717.569	693.667	70D
66-65	801 259.782(30)	801 259.796(21)	896.183	869.456	70D
67-66	813 353.706(30)	813 353.685(24)	923.314	896.183	70D

Table 6. Microwave Spectrum of  $^{16}\text{O}^{12}\text{C}^{34}\text{S}$  in the Ground Vibrational State

Transition $J' \leftarrow J''$	Observed Frequency in MHz (estimated uncertainty)	Calculated Frequency in MHz (estimated uncertainty)	Energy in $\text{cm}^{-1}$	
			Upper State	Lower State
1- 0	11 865.712(50) [67B]	11 865.671(9)	0.396	0.0
2- 1	23 731.302(15) [73A]	23 731.311(17)	1.187	0.396
3- 2	35 596.91(3) [67A]	35 596.890(24)	2.375	1.187
4- 3	47 462.40(20)[49A]	47 462.378(30)	3.958	2.375
5- 4		59 327.745(35)	5.937	3.958
6- 5		71 192.959(40)	8.312	5.937
7- 6		83 057.990(48)	11.082	8.312
8- 7		94 922.81(6)	14.248	11.082
9- 8		106 787.38(8)	17.810	14.248
10- 9	118 651.68(8)[73A]	118 651.68(11)	21.768	17.810
11-10		130 515.68(15)	26.122	21.768
12-11		142 379.34(20)	30.871	26.122
13-12		154 242.63(27)	36.016	30.871
14-13		166 105.53(34)	41.557	36.016
15-14		177 968.00(43)	47.493	41.557
16-15		189 830.02(53)	53.825	47.493
17-16		201 691.55(64)	60.553	53.825
18-17		213 552.56(77)	67.676	60.553
19-18		225 413.02(92)	75.195	67.676
20-19		237 272.91(108)	83.110	75.195
21-20		249 132.18(126)	91.420	83.110
22-21		260 990.82(146)	100.126	91.420
23-22		272 848.78 (168)	109.227	100.126
24-23		284 706.04 (192)	118.724	109.227
25-24		296 562.58(218)	128.616	118.724

Table 7. Microwave Spectrum of  $^{16}_0\text{C}^{32}\text{S}$  and  $^{18}_0\text{C}^{32}\text{S}$  in the Ground Vibrational State

Transition $J''-J'''$	$^{16}_0\text{C}^{32}\text{S}$					$^{18}_0\text{C}^{32}\text{S}$				
	Obs. Freq. in MHz (Est. Unc.)	Calc Freq. in MHz (Est. Unc.)	Energy in $\text{cm}^{-1}$		Obs. Freq. in MHz (Est. Unc.)	Calc Freq. in MHz (Est. Unc.)	Energy in $\text{cm}^{-1}$		Upper State	Lower State
1- 0	----	12 123.845(2)	0.404	0	----	11 409.717(6)	0.381	0		
2- 1	24 247.668(10) [73A]	24 247.658(4)	1.213	0.404	22 819.404(20) [73A]	22 819.406(11)	1.142	0.381		
3- 2	36 371.390(30) [73A]	36 371.410(5)	2.426	1.213	34 229.045(30) [73A]	34 229.041(16)	2.284	1.142		
4- 3	48 494.76(40) <sup>a</sup> [52C]	48 495.067(6)	4.044	2.426	----	45 638.595(20)	3.806	2.284		
5- 4	----	60 618.600(7)	6.066	4.044	----	57 048.039(23)	5.709	3.806		
6- 5	----	72 741.977(8)	8.492	6.066	----	68 457.347(24)	7.992	5.709		
7- 6	84 865.166(10) [74A]	84 865.167(9)	11.323	8.492	----	79 866.492(25)	10.656	7.992		
8- 7	----	96 988.139(9)	14.558	11.323	----	91 275.445(26)	13.701	10.656		
9- 8	----	109 110.862(9)	18.198	14.558	----	102 684.181(28)	17.126	13.701		
10- 9	121 233.301(10) [73A, 74A]	121 233.304(9)	22.242	18.198	----	114 092.672(30)	20.932	17.126		
11-10	----	133 355.434(8)	26.690	22.242	125 500.89(3) [73A]	125 500.890(42)	25.118	20.932		
12-11	----	145 477.221(7)	31.543	26.690	----	136 908.808(58)	29.685	25.118		
13-12	----	157 598.634(7)	36.800	31.543	----	148 316.400(80)	34.632	29.685		
14-13	169 719.648(10) [74A]	169 719.642(8)	42.461	36.800	----	159 723.64(11)	39.960	34.632		
15-14	181 840.209(10) [74A]	181 840.213(10)	48.526	42.461	----	171 130.49(14)	45.668	39.960		
16-15	----	193 960.317(14)	54.996	48.526	----	182 536.94(17)	51.757	45.668		
17-16	----	206 079.922(20)	61.870	54.996	----	193 942.95(22)	58.226	51.757		
18-17	----	218 198.997(26)	69.149	61.870	----	205 348.50(26)	65.076	58.226		
19-18	----	230 317.510(33)	76.831	69.149	----	216 753.56(32)	72.306	65.076		
20-19	----	242 435.432(42)	84.918	76.831	----	228 158.10(38)	79.917	72.306		
21-20	----	254 552.730(51)	93.409	84.918	----	239 562.09(44)	87.908	79.917		
22-21	----	266 669.373(62)	102.304	93.409	----	250 965.51(52)	96.279	87.908		
23-22	----	278 785.330(74)	111.603	102.304	----	262 368.34(60)	105.031	96.279		
24-23	----	290 900.570(87)	121.307	111.603	----	273 770.53(69)	114.163	105.031		
25-24	----	----	----	----	----	285 172.07(79)	123.675	114.163		
26-25	----	----	----	----	----	296 572.94(90)	133.567	123.675		

<sup>a</sup>All measurements in ref. 52C seem to be too low by about 0.2 MHz.

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Table 8. Observed microwave transitions (in MHz) for less abundant isotopes of OCS in the ground vibrational state

Isotopic Species	Transitions		Observed Frequency (estimated uncertainty)	Calculated Unsplit Frequency and Quadrupole Shifts (estimated uncertainty)	Relative Intensity of Quadrupole Components	Reference
	Upper State	Lower State				
$^{18}\text{O}^{13}\text{C}^{34}\text{S}$	J = 2	J = 1	22179.42(8)	22179.42(8)		73A
$^{18}\text{O}^{12}\text{C}^{34}\text{S}$	J = 2	J = 1	22239.850(20)	22239.850(20)		73A
$^{18}\text{O}^{13}\text{C}^{32}\text{S}$	J = 2	J = 1	22764.240(20)	22764.240(20)		73A
$^{16}\text{O}^{12}\text{C}^{36}\text{S}$	J = 2	J = 1	23198.67(10)	23198.68(10)		49B
$^{16}\text{O}^{12}\text{C}^{35}\text{S}$	J = 2	J = 1	23457.403(22)	23457.444(25) <sup>a</sup>		54B, 51A
	F = $\frac{1}{2}$	F = $\frac{1}{2}$		0.000(0)	0.083	
	F = $\frac{3}{2}$	F = $\frac{1}{2}$	23462.906(22)	5.475(20)	0.083	54B, 51A
	F = $\frac{3}{2}$	F = $\frac{3}{2}$	23453.055(22)	-4.380(16)	0.107	54B, 51A
	F = $\frac{5}{2}$	F = $\frac{3}{2}$	23456.963(22)	-0.469(2)	0.210	51A
	F = $\frac{5}{2}$	F = $\frac{5}{2}$	23462.444(22)	5.006(18)	0.090	54B, 51A
	F = 7/2	F = $\frac{5}{2}$	23456.963(22)	-0.469(2)	0.400	51A
$^{17}\text{O}^{12}\text{C}^{32}\text{S}$	J = 2	J = 1	23534.66(5)	23534.66(0)		49B, 73B
	F = $\frac{1}{2}$	F = $\frac{3}{2}$	23534.308(24)	0.079(8)	0.067	52B
	F = $\frac{3}{2}$	F = $\frac{3}{2}$	23534.481(28)	-0.091(10)	0.093	52B
	F = $\frac{5}{2}$	F = $\frac{3}{2}$	23534.101(28)	-0.279(30)	0.062	52B
	F = $\frac{3}{2}$	F = $\frac{5}{2}$		0.305(32)	0.040	52B
	F = $\frac{5}{2}$	F = $\frac{5}{2}$	23534.481(28)	0.117(12)	0.122	52B
	F = 7/2	F = $\frac{5}{2}$	23534.422(24)	0.051(5)	0.171	52B
	F = $\frac{5}{2}$	F = 7/2		-0.160(17)	0.016	52B
	F = 7/2	F = 7/2	23534.164(24)	-0.226(24)	0.095	52B
	F = 9/2	F = 7/2	23534.422(24)	0.028(3)	0.333	52B
$^{16}\text{O}^{13}\text{C}^{34}\text{S}$	J = 2	J = 1	23646.888(10)	23646.888(10)		73A
	J = 3	J = 2	35470.264(20)	35470.264(20)		73A
$^{16}\text{O}^{12}\text{C}^{33}\text{S}$	J = 2	J = 1	24019.641(20)	24019.648(20) <sup>a</sup>		51A
	F = $\frac{1}{2}$	F = $\frac{1}{2}$	24019.641(10)	0.000(0)	0.083	51A
	F = $\frac{3}{2}$	F = $\frac{1}{2}$	24012.292(10)	-7.282(8)	0.083	51A
	F = $\frac{1}{2}$	F = $\frac{3}{2}$	24032.72(2)	13.108(14)	0.017	52A
	F = $\frac{3}{2}$	F = $\frac{3}{2}$	24025.467(10)	5.826(6)	0.107	51A
	F = $\frac{5}{2}$	F = $\frac{3}{2}$	24020.264(10)	0.624(1)	0.210	51A
	F = $\frac{3}{2}$	F = $\frac{5}{2}$	24018.17(2)	-1.456(2)	0.010	52A
	F = $\frac{5}{2}$	F = $\frac{5}{2}$	24012.974(10)	-6.658(7)	0.090	51A
	F = 7/2	F = $\frac{5}{2}$	24020.264(10)	0.624(1)	0.400	51A
	J = 4	J = 3	48038.86(40) <sup>b</sup>	48039.05(5)		52C
	F = $\frac{5}{2}$	F = $\frac{3}{2}$	48038.19(40) <sup>b</sup>	-0.624(1)	0.143	52C
	F = 7/2	F = $\frac{5}{2}$	48038.19(40) <sup>b</sup>	-0.624(1)	0.191	52C
	F = 9/2	F = 7/2	48039.13(40) <sup>b</sup>	0.221(0)	0.255	52C
	F = 11/2	F = 9/2	48039.13(40) <sup>b</sup>	0.221(0)	0.333	52C
$^{16}\text{O}^{14}\text{C}^{32}\text{S}$	J = 2	J = 1	24173.0(20)	24173.0(20)		48A

<sup>a</sup>Since the original measurements in ref. 51A were calibrated with respect to  $^{16}\text{O}^{12}\text{C}^{32}\text{S}$  and  $^{16}\text{O}^{12}\text{C}^{34}\text{S}$  lines, a correction has been made for the latest estimates of their frequencies.<sup>b</sup>Data in ref. 52C are consistently low and probably should be raised by 0.2 MHz.

Table 9. Observed Microwave Transitions in Excited Vibrational States of the most Abundant Isotopic Species of Carbonyl Sulfide

Isotopic Species	Transition J' - J''	Vibrational State v <sub>1</sub> v <sub>2</sub> <sup>a</sup> v <sub>3</sub>	Observed Frequency (MHz)	Approximate Lower State Energy (cm <sup>-1</sup> )	Ref.
<sup>16</sup> O <sup>12</sup> C <sup>32</sup> S	1 0 0 4 <sup>0</sup> 0	12 229.44(8)	2105	67A	
	2 1 0 0 <sup>0</sup> 2	24 179.46(8)	1711		
	2 1 1 0 <sup>0</sup> 0	24 180.17(8)	2063		
	2 1 0 1 <sup>lc</sup> 2	24 219.54(12)	2218		
	2 1 0 1 <sup>ld</sup> 2	24 248.68(12)	2218		
	2 1 0 0 <sup>0</sup> 1	24 253.38(4)	859		
	2 1 0 1 <sup>lc</sup> 1	24 288.36(6)	1373		
	2 1 0 1 <sup>ld</sup> 1	24 315.82(6)	1373		
	2 1 0 2 <sup>0</sup> 1	24 337.50(8)	1893		
	2 1 0 3 <sup>lc</sup> 1	24 348.2(4)	2412		
	2 1 0 3 <sup>ld</sup> 1	24 400.2(4)	2412		
	2 1 0 1 <sup>lc</sup> 0	24 355.58(4)	521		
	2 1 0 1 <sup>ld</sup> 0	24 381.00(4)	521		
	2 1 0 2 <sup>0</sup> 0	24 400.79(4)	1047		
	2 1 0 3 <sup>lc</sup> 0	24 409.74(5)	1574		
	2 1 0 3 <sup>ld</sup> 0	24 459.20(5)	1574		
	3 2 1 1 <sup>lc</sup> 0	36 318.08(18)	2576		
	3 2 1 1 <sup>ld</sup> 0	36 356.78(18)	2576		
	3 2 0 1 <sup>lc</sup> 1	36 432.39(9)	1374		
	3 2 0 1 <sup>ld</sup> 1	36 473.47(9)	1374		
	3 2 0 2 <sup>2</sup> 1	36 523.38(12)	1888		
	3 2 0 1 <sup>lc</sup> 0	36 533.38(6)	522		
	3 2 0 1 <sup>ld</sup> 0	36 571.36(6)	522		
	3 2 0 2 <sup>0</sup> 0	36 601.11(6)	1048		
	3 2 0 2 <sup>2</sup> 0	36 615.23(6)	1042		
	3 2 0 5 <sup>lc</sup> 0	36 675.75(18)	2637		
	3 2 0 3 <sup>ld</sup> 0	36 704.74(18)	2637		
	3 2 0 4 <sup>2</sup> 0	36 703.77(12)	2100		
	4 3 0 0 <sup>0</sup> 1	48 506.24(40) <sup>b</sup>	861	52C	
	4 3 0 1 <sup>lc</sup> 0	48 710.80(40) <sup>b</sup>	523		
	4 3 0 1 <sup>ld</sup> 0	48 761.55(40) <sup>b</sup>	523		
	4 3 0 2 <sup>0</sup> 0	48 801.08(40) <sup>b</sup>	1049		
	4 3 0 2 <sup>2</sup> 0	48 819.92(40) <sup>b</sup>	1043		
	5 4 1 1 <sup>lc</sup> 0	60 530.2(5)	2579	67A	
	5 4 1 1 <sup>ld</sup> 0	60 594.3(5)	2579		
	5 4 0 1 <sup>lc</sup> 1	60 720.4(5)	1376		
	5 4 0 1 <sup>ld</sup> 1	60 788.3(5)	1376		
	5 4 0 2 <sup>0</sup> 1	60 843.48(15)	1895		
	5 4 0 2 <sup>2</sup> 1	60 871.68(15)	1890		

Table 9 (Continued)

5 4 0 1 <sup>lc</sup> 0	60 888.35(10)	524
5 4 0 1 <sup>ld</sup> 0	60 951.94(10)	524
5 4 0 3 <sup>ld</sup> 1	61 000.1(5)	1895
5 4 0 2 <sup>0</sup> 0	61 001.48(10)	1050
5 4 0 2 <sup>2</sup> 0	61 024.96(10)	1044
5 4 0 3 <sup>3</sup> 0	61 128.86(12)	1565
5 4 0 4 <sup>2</sup> 0	61 172.69(15)	2102
5 4 0 4 <sup>4</sup> 0	61 231.85(15)	2087
<sup>16</sup> O <sup>12</sup> C <sup>34</sup> S 2 1 0 0 <sup>0</sup> 2	23 588.44(8)	1688 67A
2 1 0 0 <sup>0</sup> 0	23 589.52(8)	2062
2 1 0 0 <sup>0</sup> 1	23 660.56(4)	847
2 1 0 1 <sup>lc</sup> 0	23 760.48(4)	519
2 1 0 1 <sup>ld</sup> 0	23 784.74(4)	519
2 1 0 2 <sup>0</sup> 0	23 804.97(4)	1045
3 2 0 0 <sup>0</sup> 1	35 490.77(6)	848
3 2 0 1 <sup>lc</sup> 0	35 640.66(6)	520
3 2 0 1 <sup>ld</sup> 0	35 676.98(6)	520
3 2 0 2 <sup>0</sup> 0	35 707.50(6)	1046
3 2 0 2 <sup>2</sup> 0	35 720.27(6)	1040
<sup>16</sup> O <sup>13</sup> C <sup>32</sup> S 2 1 0 0 <sup>0</sup> 2	24 102.54(4)	1702 73A
2 1 1 0 <sup>0</sup> 0	24 110.60(10)	2010
2 1 0 0 <sup>0</sup> 1	24 175.751(20)	855
2 1 0 1 <sup>lc</sup> 1	24 208.276(40)	1353
2 1 0 1 <sup>ld</sup> 1	24 236.538(40)	1353
2 1 0 2 <sup>0</sup> 1	24 254.68(5)	1857
2 1 0 1 <sup>lc</sup> 0	24 274.60(5)	505
2 1 0 1 <sup>ld</sup> 0	24 300.64(5)	505
2 1 0 2 <sup>0</sup> 0	24 316.962(20)	1017
2 1 0 3 <sup>lc</sup> 0	24 322.92(40)	1528
2 1 0 3 <sup>ld</sup> 0	24 373.26(5)	1528
2 1 0 4 <sup>0</sup> 0	24 368.76(10)	2044
3 2 0 0 <sup>0</sup> 2	36 153.67(10)	1703
3 2 1 0 <sup>0</sup> 0	36 165.72(10)	2010
3 2 0 0 <sup>0</sup> 1	36 263.46(10)	856
3 2 0 2 <sup>2</sup> 1	36 400.79(10)	1851
3 2 0 1 <sup>ld</sup> 0	36 450.876(20)	506
3 2 0 2 <sup>0</sup> 0	36 475.38(10)	1017
3 2 0 3 <sup>lc</sup> 0	36 494.348(30)	1529
3 2 0 3 <sup>ld</sup> 0	36 559.81(10)	1529
3 2 0 2 <sup>2</sup> 0	36 490.723(40)	1011

Table 9 (Continued)

5 4	0 3 <sup>3</sup> 0	60 915.415(20)	1521
5 4	0 3 <sup>1d</sup> 0	60 932.540(25)	1531
5 4	0 4 <sup>2</sup> 0	60 950.15(6)	2041
5 4	0 4 <sup>4</sup> 0	61 012.39(9)	2026
10 9	0 0 <sup>0</sup> 1	120 873.34(5)	873
10 9	0 2 <sup>0</sup> 0	121 580.46(7)	1034
10 9	0 2 <sup>2c</sup> 0	121 629.93(10)	1028
10 9	0 2 <sup>2d</sup> 0	121 630.78(10)	1028
 <sup>18</sup> O <sup>12</sup> C <sup>32</sup> S	 2 1	 22 679.38(8)	 2025 73A
2 1	0 0 <sup>0</sup> 2	22 688.524(40)	1680
2 1	0 0 <sup>0</sup> 1	22 754.570(20)	845
2 1	0 1 <sup>lc</sup> 1	22 788.585(40)	1355
2 1	0 1 <sup>ld</sup> 1	22 812.773(40)	1355
2 1	0 2 <sup>0</sup> 1	22 035.26(10)	1865
2 1	0 1 <sup>lc</sup> 0	22 848.653(20)	515
2 1	0 1 <sup>ld</sup> 0	22 871.228(20)	515
2 1	0 2 <sup>0</sup> 0	22 891.663(20)	1035
2 1	0 3 <sup>1c</sup> 0	22 902.513(30)	1555
2 1	0 3 <sup>1d</sup> 0	22 946.543(40)	1555
2 1	0 4 <sup>0</sup> 0	22 947.972(40)	2081
3 2	0 0 <sup>0</sup> 1	34 131.83(10)	845
3 2	0 1 <sup>lc</sup> 1	34 182.85(15)	1355
3 2	0 1 <sup>ld</sup> 1	34 219.151(30)	1355
3 2	0 2 <sup>0</sup> 1	34 252.84(7)	1865
3 2	0 2 <sup>2</sup> 1	34 268.13(10)	1860
3 2	0 1 <sup>lc</sup> 0	34 272.920(25)	515
3 2	0 1 <sup>ld</sup> 0	34 306.73(10)	515
3 2	0 2 <sup>0</sup> 0	34 337.45(10)	1035
3 2	0 2 <sup>2</sup> 0	34 350.073(25)	1030
3 2	0 3 <sup>1c</sup> 0	34 353.748(40)	1555
3 2	0 3 <sup>1d</sup> 0	34 419.83(15)	1555
3 2	0 4 <sup>0</sup> 0	34 421.89(15)	2082
5 4	0 3 <sup>3</sup> 0	57 349.313(30)	1545
5 4	0 4 <sup>2</sup> 0	57 394.56(8)	2080
5 4	0 4 <sup>4</sup> 0	57 447.96(10)	2065
11 10	0 0 <sup>0</sup> 1	125 144.13(8)	860
11 10	0 2 <sup>2</sup> 1	125 642.98(15)	1875
11 10	0 1 <sup>lc</sup> 0	125 661.45(3)	533
11 10	0 2 <sup>0</sup> 0	125 898.90(13)	1053
11 10	0 2 <sup>2c</sup> 0	125 943.69(4)	1048
11 10	0 2 <sup>2d</sup> 0	125 944.57(3)	1048
11 10	0 3 <sup>3</sup> 0	126 162.98(7)	1560
11 10	0 4 <sup>4</sup> 0	126 380.09(20)	2080

<sup>a</sup>Note that these tables use a different vibrational numbering from that used in the primary references (see explanation in the Introduction).

<sup>b</sup>Data in ref. 52C are consistently low and should be raised by about 0.2 MHz.

Table 10. Observed microwave transitions in excited vibrational states of less abundant species of OCS.

Isotopic Species	Transition	Vibrational State			Observed Frequency (MHz)	Ref.		
		Upper State	Lower State	$v_1$	$v_2$	$v_3$		
<sup>18</sup> O <sup>12</sup> C <sup>34</sup> S	J=2 $\leftarrow$ J=1			0	0 <sup>0</sup>	1	22176.76(3)	73A
	J=2 $\leftarrow$ J=1			0	1 <sup>lc</sup>	0	22268.57(5)	
	J=2 $\leftarrow$ J=1			0	1 <sup>ld</sup>	0	22290.14(5)	
	J=2 $\leftarrow$ J=1			0	2 <sup>0</sup>	0	22310.87(6)	
<sup>18</sup> O <sup>13</sup> C <sup>32</sup> S	J=2 $\leftarrow$ J=1			0	0 <sup>0</sup>	1	22699.94(15)	73A
	J=2 $\leftarrow$ J=1			0	1 <sup>lc</sup>	0	22790.88(8)	
	J=2 $\leftarrow$ J=1			0	1 <sup>ld</sup>	0	22814.034(60)	
	J=3 $\leftarrow$ J=2			0	1 <sup>ld</sup>	0	34221.116(60)	
<sup>16</sup> O <sup>13</sup> C <sup>34</sup> S	J=2 $\leftarrow$ J=1			0	0 <sup>0</sup>	1	23576.55(3)	73A
	J=2 $\leftarrow$ J=1			0	1 <sup>lc</sup>	0	23673.41(6)	73B
	J=2 $\leftarrow$ J=1			0	1 <sup>ld</sup>	0	23698.20(6)	73B
	J=3 $\leftarrow$ J=2			0	2 <sup>0</sup>	0	35573.06(4)	73A
<sup>16</sup> O <sup>12</sup> C <sup>33</sup> S	J=2 $\leftarrow$ J=1			0	0 <sup>0</sup>	1	23947.4(10)	68B
	J=2 $\leftarrow$ J=1			0	1 <sup>lc</sup>	0	24049.4(10)	
	F=5/2 $\leftarrow$ F=3/2			0	1 <sup>lc</sup>	0	24044.0(10)	
	F=5/2 $\leftarrow$ F=5/2			0	1 <sup>lc</sup>	0	24046.9(10)	
<sup>16</sup> O <sup>12</sup> C <sup>32</sup> S	F=7/2 $\leftarrow$ F=5/2			0	1 <sup>lc</sup>	0	24051.2(10)	
	J=2 $\leftarrow$ J=1			0	1 <sup>ld</sup>	0	24074.2(10)	
	F=5/2 $\leftarrow$ F=3/2			0	1 <sup>ld</sup>	0	24069.2(10)	
	F=5/2 $\leftarrow$ F=5/2			0	1 <sup>ld</sup>	0	24072.0(10)	
<sup>16</sup> O <sup>12</sup> C <sup>31</sup> S	F=3/2 $\leftarrow$ F=3/2			0	1 <sup>ld</sup>	0	24072.0(10)	
	F=3/2 $\leftarrow$ F=5/2			0	1 <sup>ld</sup>	0	24075.7(10)	
	J=2 $\leftarrow$ J=1			0	2 <sup>0</sup>	0	24092.4(10)	

<sup>a</sup>Note that these tables use a different vibrational numbering from that used in the primary references (see explanation in the Introduction).

Table 11.  $\lambda$ -doublet Transitions (in MHz) in the Bending Vibrational State ( $v_2$ )<sup>a</sup>

	$^{16}_0\text{C}^{32}\text{S}$ [ref. 67C,72B]		$^{16}_0\text{C}^{32}\text{S}$ [ref. 67C,73C]		$^{18}_0\text{C}^{32}\text{S}$ [ref. 73A,73C]	
	Observed (Uncertainty)	Calculated (Uncertainty)	Observed (Uncertainty)	Calculated (Uncertainty)	Observed (Uncertainty)	Calculated (Uncertainty)
1	12.722 88(10)	12.722 81(0)	13.015 92(50)	13.015 67(1)	11.306 55(50)	11.305 99(2)
2	38.168 36(10)	38.168 32(1)	39.046 83(50)	39.046 89(3)	33.917 95(100)	33.917 89(6)
3	76.336 32(10)	76.336 34(2)	78.093 36(50)	78.093 46(5)	67.835 50(100)	67.835 51(12)
4	127.226 48(10)	127.226 55(2)	130.154 95(50)	130.155 04(8)	113.058 50(100)	113.058 61(19)
5	190.838 50(10)	190.838 54(4)	195.231 06(50)	195.231 21(10)	169.586 85(100)	169.586 84(28)
6	267.171 86(10)	267.171 80(4)	273.321 35(50)	273.321 44(11)	237.419 75(100)	237.419 77(39)
7	356.225 85(100)	356.225 72(4)	364.425 17(50)	364.425 07(13)	316.556 85(100)	316.556 88(52)
8	457.999 60(10)	457.999 57(5)	468.541 43(50)	468.541 35(18)	----	406.997 56(66)
9	572.492 46(20)	572.492 55(6)	----	585.669 42(30)	----	508.741 14(84)
10	699.703 55(20)	699.703 72(8)	----	715.808 31(50)	----	621.786 83(105)
11	839.632 20(20)	839.632 06(12)	----	858.956 95(80)	----	746.133 78(132)
12	992.276 00(200)	992.276 45(20)	----	1 015.114 16(120)	----	881.781 05(166)
35	8 008.57(20)	8 008.616(14)	8 192.77(20)	8 192.798(36)	----	7 117.137(44)
36	8 465.84(20)	8 465.844(15)	8 660.53(20)	8 660.533(36)	----	7 523.494(46)
37	8 935.76(20)	8 935.727(17)	9 141.17(20)	9 141.213(35)	----	7 941.100(47)
38	9 418.21(20)	9 418.261(18)	9 634.86(20)	9 634.835(34)	8 369.97(14)	8 369.954(48)
39	9 913.34(20)	9 913.443(20)	10 141.34(20)	10 141.393(33)	8 810.00(14)	8 810.051(48)
40	10 421.23(20)	10 421.268(22)	10 660.91(20)	10 660.885(33)	9 261.36(14)	9 261.390(48)
41	10 941.70(20)	10 941.732(25)	11 193.26(20)	11 193.306(37)	----	9 723.966(47)
42	11 474.84(20)	11 474.832(28)	11 738.66(20)	11 738.652(44)	10 197.81(14)	10 197.777(46)
43	12 020.52(20)	12 020.563(31)	----	12 296.918(56)	----	10 682.819(44)
44	12 578.89(20)	12 578.921(35)	12 868.15(20)	12 868.101(72)	11 179.10(20)	11 179.088(42)
45	13 149.92(20)	13 149.902(40)	----	13 452.195(93)	11 686.59(20)	11 686.581(42)
46	13 733.48(20)	13 733.500(46)	----	14 049.196(118)	----	12 205.295(44)
47	14 329.70(20)	14 329.711(52)	----	14 659.100(149)	12 735.24(14)	12 735.226(50)
48	14 938.59(20)	14 938.531(59)	----	15 281.901(185)	13 276.41(14)	13 276.370(61)
49	15 559.98(20)	15 559.955(68)	----	15 917.59(23)	----	13 828.724(76)
50	16 194.00(20)	16 193.978(77)	----	16 566.18(28)	14 392.20(20)	14 392.284(97)

<sup>a</sup>The  $v_2$  vibrational states are at 520.41 cm<sup>-1</sup> for  $^{16}_0\text{C}^{32}\text{S}$  [ref. 72A], 505.16 cm<sup>-1</sup> for  $^{16}_0\text{C}^{32}\text{S}$  [ref. 71A], and about 515 cm<sup>-1</sup> for  $^{18}_0\text{C}^{32}\text{S}$ .

Table 12. Low Frequency  $\Delta$ -doublet Transitions  
for  $^{16}\text{O}^{12}\text{C}^{34}\text{S}$  in the Bending Vibrational  
State ( $v_2$ )<sup>a</sup>. [Ref. 73C]

J	Obs. Freq. (kHz) (Est. Uncertainty)	Calc. Freq. (kHz) (Est. Uncertainty)
1	12 137.73(20)	12 137.589(13)
2	36 412.73(20)	36 412.672(34)
3	72 825.07(20)	72 825.06(6)
4	121 374.46(20)	121 374.47(7)
5	182 060.49(20)	182 060.53(8)
6	254 882.78(20)	254 882.77(10)
7	339 840.58(200)	339 840.61(22)
8	436 933.48(100)	436 933.40(46)

<sup>a</sup>The  $v_2$  vibrational state is  $519 \text{ cm}^{-1}$  above the ground state.

### 2.3. OCS References

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## 3. Hydrogen Cyanide

### 3.1. Organization of the Spectral Tables

Although hydrogen cyanide has a very sparse spectrum in the microwave region because of its very large *B* value (or small moment of inertia), a great many microwave transitions have been recorded for vibrationally excited hydrogen cyanide primarily due to transitions between the nearly degenerate doublet levels in the bending vibrational states. Tables 19 through 23 list observed frequencies for such transitions between doublet levels. Since table 19 contains the strongest of these doublet transitions, the calculated transitions through *J* = 22 have also been included in that table.

For the ground vibrational state table 13 gives the measured rotational constants and table 16 gives both the measured and the calculated transitions through 300 GHz. In table 16 the splitting due to the nuclear quadrupole moment of the nitrogen is given, but further splitting (such as due to the deuterium quadrupole) are ignored. The effect of the deuterium quadrupole splitting is shown in table 17 where the observed hyperfine measurements for DCN are given.

### 3.2. Hydrogen Cyanide Spectral Tables

Table 13. Rotational Constants for Hydrogen Cyanide

Molecular Species	<i>B</i> <sub>0</sub> (MHz)	<i>D</i> <sub>0</sub> (kHz)	Ref.
H <sup>12</sup> C <sup>14</sup> N	44 315.9757(4)	87.24(6)	[69A]
H <sup>13</sup> C <sup>14</sup> N	43 170.09(6)	83.0 <sup>a</sup>	[71A]
H <sup>12</sup> C <sup>15</sup> N	43 027.69(5)	82.3 <sup>a</sup>	[71A]
D <sup>12</sup> C <sup>14</sup> N	36 207.4627(2)	57.83(4)	[69A]
D <sup>13</sup> C <sup>14</sup> N	35 587.62(5)	55.7 <sup>a</sup>	[71A]
D <sup>12</sup> C <sup>15</sup> N	35 169.85(5)	54.5 <sup>a</sup>	[71A]

#### Structure

linear

$$r_e \text{ (C-N)} 1.15321 \pm 0.00010 \text{ \AA} [71A]$$

$$r_e \text{ (C-H)} 1.0655 \pm 0.0005 \text{ \AA} [71A]$$

<sup>a</sup>Calculated values taken from ref. [69B].

Table 14. Hyperfine constants and dipole moment for hydrogen cyanide

Molecule Vib. State Transition Measured	DCN 000 J = 1-0	$D^{13}C^{14}N$ 000 J = 1-0	HCN 000 J = 1-0	HCN 010 J = 2-1	HCN 020 J = 1-0	HCN 0220 J = 3-2	HCN 000 J = 1-0
$\mu$ (Debyes)	2.990198(1500) [70C]	----	2.984594(1500) <sup>a</sup> [70C]	2.941642(1500) [70C]	2.89865(150) [70C]	2.89813(150) [70C]	----
$\mu$	1.0018776(70) [70C]	----	----	0.9856088(80) [70C]	0.971204(36) [70C]	0.97103(17) [70C]	----
$\mu(H^{13}C^{14}N)$	202.23(50) [70C]	----	----	----	----	----	----
(eqQ) <sub>D</sub> (kHz)	-4703.96(47) [70C]	----	-4707.89(8) [70C]	-4807.9(19) [70C]	-4899.0(21) [70C]	----	----
(eqQ) (kHz)	-4703.96(47) [70C]	----	----	395.1(27) [70C]	----	----	----
eqQ  <sub>H</sub> (kHz)	----	----	10.13(3) [70C]	12.07(27) [70C]	10.70(78) [70C]	----	----
C <sub>H</sub> (kHz)	8.23(18) [70C]	----	----	----	----	----	----
C <sub>D</sub> or C <sub>H</sub> (kHz)	-0.57(25) [70C]	----	-4.32(7) [70C]	-27.4(55) [70C]	-3.8(15) [70C]	----	----
C <sub>13</sub> <sup>b</sup> (kHz)	----	15.0(20) [73C]	----	----	----	----	----
S <sub>HN</sub> (kHz)	----	----	0.154(19) [70C]	----	----	----	----
B <sub>z</sub>	----	----	-0.0980(40) [73A]	-0.100(2) <sup>b</sup> [70A]	----	----	-0.0904(6) [73B]
B <sub>  </sub>	----	----	----	+0.38(12) <sup>b</sup> [70A]	----	----	----
X <sub>z</sub> X <sub>  </sub> (erg/G <sup>2</sup> ·mole)	----	----	----	----	----	----	7.2(8)×10 <sup>-6</sup> [73B]
Q <sub>  </sub> (esu)	----	----	----	----	----	----	3.1(12)×10 <sup>-26</sup> [73B]

<sup>a</sup>Polarity determined to be <sup>+</sup>HNC<sup>-</sup> [73A].<sup>b</sup>Relative signs were fixed in ref. 70A while absolute signs were fixed by ref. 73B and 73A.

Table 15. Rotational constants for the lower vibrational states of hydrogen cyanide.

Isotopic Species	Vibrational <sup>c</sup> State			B <sub>v</sub> (MHz)	q <sub>v</sub> (kHz)
	v <sub>1</sub>	v <sub>2</sub> <sup>l</sup>	v <sub>3</sub>		
<sup>12</sup> H <sup>12</sup> C <sup>14</sup> N <sup>a</sup>	0	1 <sup>1</sup>	0	44 422.437±0.030 [71A]	224 476.57±0.30 - 2.65865(±0.00292)J(J+1) + 3.602(±0.620)×10 <sup>-5</sup> J <sup>2</sup> (J+1) <sup>2</sup> [67A]
	0	2 <sup>0</sup>	0	44 544.033±0.060 [71A]	----
	0	3 <sup>1</sup>	0	----	231 120.0±4.0 - 2.98(±0.09)J(J+1) + 3.6×10 <sup>-5</sup> J <sup>2</sup> (J+1) <sup>2</sup> [67A]
	0	0 <sup>0</sup>	1	44 013.775±0.100 [71A]	----
<sup>13</sup> H <sup>13</sup> C <sup>14</sup> N	0	1 <sup>1</sup>	0	----	214 837.4±1.4 - 2.436 (±0.017)J(J+1) [61A]
<sup>12</sup> H <sup>12</sup> C <sup>15</sup> N	0	1 <sup>1</sup>	0	----	211 938.1±5.2 - 2.392 (±0.072)J(J+1) [61A]
<sup>12</sup> D <sup>12</sup> C <sup>14</sup> N <sup>b</sup>	0	1 <sup>1</sup>	0	36 337.037±0.030 [71A]	186 191.58±0.50 - 2.20697(±0.00380)J(J+1) + 4.790(±0.620)×10 <sup>-5</sup> J <sup>2</sup> (J+1) <sup>2</sup> [67A]
	0	2 <sup>0</sup>	0	36 474.259±0.050 [71A]	----
	0	3 <sup>1</sup>	0	----	190 916.±2.0 - 2.44(±0.02)J(J+1) + 4.8×10 <sup>-5</sup> J <sup>2</sup> (J+1) <sup>2</sup> [67A]
	0	0 <sup>0</sup>	1	36 011.116±0.100 [71A]	----
<sup>12</sup> D <sup>13</sup> C <sup>14</sup> N	0	1 <sup>1</sup>	0	----	182 294.2±1.2 - 2.082 (±0.012)J(J+1) [61A]
	0	2 <sup>0</sup>	0	35 833.92 ±0.20 [71A]	----
<sup>12</sup> D <sup>12</sup> C <sup>15</sup> N	0	1 <sup>1</sup>	0	----	176 079.9±2.2 - 2.019 (±0.022)J(J+1) [61A]
	0	2 <sup>0</sup>	0	35 427.09±0.15 [71A]	----

<sup>a</sup>For H<sup>12</sup>C<sup>14</sup>N q<sub>v</sub> (MHz) = 221.1550 + 2.10 v<sub>1</sub> + 3.3215 v<sub>2</sub> - 0.03 v<sub>3</sub> - (0.002495 + 0.000163 v<sub>2</sub>) J(J+1) + 3.6×10<sup>-8</sup>J<sup>2</sup>(J+1)<sup>2</sup> [67A, 69B] and D<sub>v</sub> (kHz) = 87.24 - 0.83 v<sub>1</sub> + 2.13 v<sub>2</sub> + 0.22 v<sub>3</sub> [71A, 69B].<sup>b</sup>For D<sup>12</sup>C<sup>14</sup>N q<sub>v</sub> (MHz) = 183.8294 - 4.41 v<sub>1</sub> + 2.3622 v<sub>2</sub> + 4.53 v<sub>3</sub> - (0.002089 + 0.000118 v<sub>2</sub>) J(J+1) + 4.8×10<sup>-8</sup>J<sup>2</sup>(J+1)<sup>2</sup> [67A, 69B] and D<sub>v</sub> (kHz) = 57.83 - 0.27 v<sub>1</sub> + 2.10 v<sub>2</sub> - 0.03 v<sub>3</sub> [71A, 69B].<sup>c</sup>Note that these tables use a different vibrational numbering from that used in the primary references (see explanation in the Introduction).

Table 16. Microwave spectrum of various isotopes of HCN in the ground vibrational state

Isotopic Species	Transition		Observed Freq. (MHz) (estimated uncertainty)	Calculated Unsplit Frequency (MHz) and Quadrupole Shifts (estimated uncertainty)	Relative Intensity of Quadrupole Components	Ref.
$\text{H}^{12}\text{C}^{14}\text{N}$	J = 1	J = 0	88 631.6024(10)	88 631.6024(10)		
	$F_{\text{N}}=2$	$F_{\text{N}}=1$	88 631.8473(10)	0.2455(0)	0.555	[69A]
	$F_{\text{N}}=1$	$F_{\text{N}}=1$	88 630.4157(10)	-1.1871(0)	0.333	[69A]
	$F_{\text{N}}=0$	$F_{\text{N}}=1$	88 633.9360(10)	2.3337(0)	0.111	[69A]
	J = 2	J = 1	177 261.1112(20)	177 261.1112(20)		
	$F_{\text{N}}=3$	$F_{\text{N}}=2$	177 261.2232(20)	0.1110(0)	0.466	[69A]
	$F_{\text{N}}=2$	$F_{\text{N}}=2$	177 259.6767(20)	-1.4326(0)	0.083	[69A]
	$F_{\text{N}}=1$	$F_{\text{N}}=2$	----	0.9011(0)	0.006	
	$F_{\text{N}}=2$	$F_{\text{N}}=1$	177 261.1104(20)	0.0000(0)	0.250	[69A]
	$F_{\text{N}}=1$	$F_{\text{N}}=1$	177 263.4450(20)	2.3337(0)	0.083	[69A]
	$F_{\text{N}}=1$	$F_{\text{N}}=0$	177 259.9233(20)	-1.1871(0)	0.111	[69A]
	J = 3	J = 2	265 886.18(55)	265 886.432(10)		[56D]
	$F_{\text{N}}=4$	$F_{\text{N}}=3$		0.066(0)	0.429	
	$F_{\text{N}}=3$	$F_{\text{N}}=3$		-1.543(0)	0.037	
	$F_{\text{N}}=2$	$F_{\text{N}}=3$		0.545(0)	0.001	
	$F_{\text{N}}=3$	$F_{\text{N}}=2$		0.000(0)	0.296	
	$F_{\text{N}}=2$	$F_{\text{N}}=2$		2.089(0)	0.037	
	$F_{\text{N}}=2$	$F_{\text{N}}=1$		-0.245(0)	0.200	
$\text{H}^{13}\text{C}^{14}\text{N}$	J = 1	J = 0	86 339.86(10)	86 339.86(10)		[71A]
	$F_{\text{N}}=2$	$F_{\text{N}}=1$	86 340.05(10)	0.245(1)	0.555	[71A]
	$F_{\text{N}}=1$	$F_{\text{N}}=1$	86 338.75(10)	-1.187(2)	0.333	[71A]
	$F_{\text{N}}=0$	$F_{\text{N}}=1$	86 342.16(10)	2.334(2)	0.111	[71A]
	J = 2	J = 1		172 680.04(21)		
	$F_{\text{N}}=3$	$F_{\text{N}}=2$		0.111(1)	0.466	
	$F_{\text{N}}=2$	$F_{\text{N}}=2$		-1.432(2)	0.083	
	$F_{\text{N}}=2$	$F_{\text{N}}=1$		0.000(0)	0.250	
	$F_{\text{N}}=1$	$F_{\text{N}}=1$		2.334(2)	0.083	
	$F_{\text{N}}=1$	$F_{\text{N}}=0$		-1.187(2)	0.111	
	J = 3	J = 2		259 011.58(55)		
	$F_{\text{N}}=4$	$F_{\text{N}}=3$		0.066(1)	0.429	
	$F_{\text{N}}=3$	$F_{\text{N}}=3$		-1.543(2)	0.037	
	$F_{\text{N}}=3$	$F_{\text{N}}=2$		0.000(0)	0.296	
	$F_{\text{N}}=2$	$F_{\text{N}}=2$		2.089(2)	0.037	
	$F_{\text{N}}=2$	$F_{\text{N}}=1$		-0.245(1)	0.200	
$\text{HC}^{15}\text{N}$	J = 1	J = 0	86 055.05(10)	86 055.05(10)		[71A]
	J = 2	J = 1		172 108.12(20)		
	J = 3	J = 2		258 157.25(30)		
$\text{D}^{12}\text{C}^{14}\text{N}$	J = 1	J = 0	72 414.6941(7)	72 414.6941(7)		[69A]
	$F_{\text{N}}=2$	$F_{\text{N}}=1$		0.2434(2)	0.555	
	$F_{\text{N}}=1$	$F_{\text{N}}=1$		-1.1842(2)	0.333	
	$F_{\text{N}}=0$	$F_{\text{N}}=1$		2.3355(2)	0.111	
	J = 2	J = 1	144 828.0003(15)	144 828.0003(15)		[69A]
	$F_{\text{N}}=3$	$F_{\text{N}}=2$		0.1090(2)	0.466	
	$F_{\text{N}}=2$	$F_{\text{N}}=2$		-1.4276(2)	0.083	
	$F_{\text{N}}=2$	$F_{\text{N}}=1$		0.0000(0)	0.250	
	$F_{\text{N}}=1$	$F_{\text{N}}=1$		2.3355(2)	0.083	
	$F_{\text{N}}=1$	$F_{\text{N}}=0$		-1.1842(2)	0.111	

Table 16. (Continued)

	$J = 3$	$J = 2$	217 238.40(45)	217 238.531(10)	[56D]
	$F_N = 4$	$F_N = 3$		0.064(1)	0.429
	$F_N = 3$	$F_N = 2$		0.000(0)	0.296
	$F_N = 2$	$F_N = 1$		-0.243(1)	0.200
	$J = 4$	$J = 3$	289 644.67(60)	289 644.897(20)	[56D]
	$F_N = 5$	$F_N = 4$		0.044(1)	0.407
	$F_N = 4$	$F_N = 3$		0.000(0)	0.313
	$F_N = 3$	$F_N = 2$		-0.109(1)	0.238
$D^{13}CN$	$J = 1$	$J = 0$	71 175.01(10)	71 175.0(10)	
	$F_N = 2$	$F_N = 1$	71 175.22(10)	0.243(2)	0.555 [71A]
	$F_N = 1$	$F_N = 0$	71 173.89(10)	-1.184(3)	0.333 [71A]
	$F_N = 0$	$F_N = 1$	71 177.36(10)	2.336(4)	0.111 [71A]
	$J = 2$	$J = 1$		142 348.68(20)	
	$F_N = 3$	$F_N = 2$		0.109(2)	0.466
	$F_N = 2$	$F_N = 1$		-1.428(3)	0.083
	$F_N = 2$	$F_N = 1$		0.000(0)	0.250
	$F_N = 1$	$F_N = 0$		2.336(4)	0.083
	$F_N = 1$	$F_N = 0$		-1.184(3)	0.111
	$J = 3$	$J = 2$		213 519.68(30)	
	$F_N = 4$	$F_N = 3$		0.064(2)	0.429
	$F_N = 3$	$F_N = 2$		0.000(0)	0.296
	$F_N = 2$	$F_N = 1$		-0.243(2)	0.200
	$J = 4$	$J = 3$		284 686.67(40)	
	$F_N = 5$	$F_N = 4$		0.044(2)	0.407
	$F_N = 4$	$F_N = 3$		0.000(0)	0.313
	$F_N = 3$	$F_N = 2$		-0.109(2)	0.238
$D^{12}C^{15}N$	$J = 1$	$J = 0$	70 339.48(10)	70 339.48(10)	[71A]
	$J = 2$	$J = 1$		140 677.65(20)	
	$J = 3$	$J = 2$		211 013.21(30)	
	$J = 4$	$J = 3$		281 344.84(40)	

Table 17. Hyperfine measurements for ground state transitions of DCN using a beam maser. [Ref. 69A]

Transition			Observed Freq. (MHz)	Calc. Freq. (MHz)	Relative Intensity
$J=1-0$	$F_N = 1-1$	$F=1-0, 1, 2$	72 413.484 3	72 413.483 7	11
		$F=2-1, 2$	72 413.514 3	72 413.514 1	18
		$F=0-0, 1$	72 413.558 4	72 413.559 2	4
$F_N = 2-1$	$F=1-0, 1, 2$	72 414.905 4	72 414.905 8	11	
	$F=2-1, 2$	72 414.927 0	72 414.927 3	18	
	$F=3-2$	72 414.973 2	72 414.972 4	26	
$F_N = 0-1$	$F=1-0, 1, 2$	72 417.029 7	72 417.029 7	11	
$J=2-1$	$F_N = 1-0$	$F=1-1$	144 826.841 4	144 826.841 2	33
		$F=2-1$	144 826.809 7	144 826.809 9	55

Table 18. Microwave transitions observed for different isotopic species of HCN in vibrationally excited states [Ref. 71A]

Molecule	Vibrational <sup>a</sup>			Transition	Observed Frequency	Relative Intensity of Quadrupole Components	Energy of Lower State in cm <sup>-1</sup>
	v <sub>1</sub>	v <sub>2</sub>	v <sub>3</sub>	Upper State	Lower State		
H <sup>12</sup> C <sup>14</sup> N	0	0 <sup>0</sup>	1	J=1	J=0	88 027.20(20)	2097
	0	2 <sup>0</sup>	0	J=1	J=0	89 087.70(12) <sup>b</sup>	1411
				F <sub>N</sub> =1	F <sub>N</sub> =1	89 086.53(15)	33
				F <sub>N</sub> =2	F <sub>N</sub> =1	89 087.92(10)	56
				F <sub>N</sub> =0	F <sub>N</sub> =1	89 090.13(15)	11
	0	1 <sup>1c</sup>	0	J=2	J=1	177 238.71(10) <sup>b</sup>	715
				F <sub>N</sub> =2	F <sub>N</sub> =1	177 237.45(15)	25
				F <sub>N</sub> =1	F <sub>N</sub> =1	177 238.96(10)	55
				F <sub>N</sub> =1	F <sub>N</sub> =0	177 240.65(15)	11
	0	1 <sup>1d</sup>	0	J=2	J=1	178 136.50(10) <sup>b</sup>	715
				F <sub>N</sub> =2	F <sub>N</sub> =1	178 135.25(15)	25
				F <sub>N</sub> =1	F <sub>N</sub> =1	178 136.76(10)	55
				F <sub>N</sub> =1	F <sub>N</sub> =0	178 138.37(15)	11
D <sup>12</sup> C <sup>14</sup> N	0	0 <sup>0</sup>	1	J=1	J=0	72 022.00(20)	1925
	0	2 <sup>0</sup>	0	J=1	J=0	72 948.27(10) <sup>b</sup>	1130
				F <sub>N</sub> =1	F <sub>N</sub> =1	72 947.16(10)	33
				F <sub>N</sub> =2	F <sub>N</sub> =1	72 948.48(10)	56
				F <sub>N</sub> =0	F <sub>N</sub> =1	72 950.57(10)	11
	0	1 <sup>1c</sup>	0	J=2	J=1	144 974.39(10) <sup>b</sup>	572
				F <sub>N</sub> =2	F <sub>N</sub> =1	144 973.18(15)	25
				F <sub>N</sub> =1	F <sub>N</sub> =1	144 974.64(10)	55
				F <sub>N</sub> =1	F <sub>N</sub> =0	144 976.17(10)	11
	0	1 <sup>1d</sup>	0	J=2	J=1	145 719.03(10) <sup>b</sup>	572
				F <sub>N</sub> =2	F <sub>N</sub> =1	145 717.85(15)	25
				F <sub>N</sub> =1	F <sub>N</sub> =1	145 719.28(10)	55
				F <sub>N</sub> =1	F <sub>N</sub> =0	145 720.76(10)	11
	0	2 <sup>0</sup>	0	J=2	J=1	145 891.34(10) <sup>b</sup>	1133
				F <sub>N</sub> =2	F <sub>N</sub> =2	145 889.98(15)	19
				F <sub>N</sub> =1	F <sub>N</sub> =0		
				F <sub>N</sub> =2	F <sub>N</sub> =1	145 891.42(10)	72
				F <sub>N</sub> =3	F <sub>N</sub> =2		
D <sup>13</sup> C <sup>14</sup> N	0	2 <sup>0</sup>	0	J=1	J=0	71 667.6(4)	1121
D <sup>12</sup> C <sup>15</sup> N	0	2 <sup>0</sup>	0	J=1	J=0	70 853.95(30)	1131

<sup>a</sup>Note that these tables use a different vibrational numbering from that used in the primary references (see explanation in the Introduction).

<sup>b</sup>Frequencies calculated from measured quadrupole transitions.

Table 19.  $\Delta$ -Doublet Transitions for HCN and DCN in the Bending Vibrational State ( $\nu_2$ )

J	Observed Frequency (estimated uncertainty)	HCN Calculated Frequency (estimated uncertainty)	Ref.	Observed Frequency (estimated uncertainty)	DCN Calculated Frequency (estimated uncertainty)	Ref.	J
1	448.9431(8)	448.9425(6)	70B	...	372.3743(10)		1
2	1 346.758(12)	1 346.7637(17)	56B	...	1 117.0700(29)		2
3	2 693.349(20)	2 693.3360(32)	56B	...	2 233.981(6)		3
4	4 488.475(40)	4 488.4682(49)	56B	3 722.98(4)	3 722.949(9)	56A	4
5	6 731.89(3)	6 731.9053(68)	56B, 61A	5 583.85(4)	5 583.762(12)	56A	5
6	9 423.32(2)	9 423.329(8)	61A	7 816.18(4)	7 816.157(15)	56A, 61A	6
7	12 562.32(3)	12 562.357(10)	61A	10 419.81(4)	10 419.81(4)	56C, 61A	7
8	16 148.55(5)	16 148.544(11)	61A	13 394.36(3)	13 394.371(20)	67A	8
9	20 181.40(5)	20 181.382(12)	61A	16 739.39(3)	16 739.401(22)	67A	9
10	24 660.31(4)	24 660.301(14)	67A	20 454.40(5)	20 454.433(23)	61A	10
11	29 584.66(4)	29 584.666(16)	67A	24 538.92(5)	24 538.944(23)	61A	11
12	34 953.76(5)	34 953.781(20)	67A	28 992.37(4)	28 992.360(24)	67A	12
13	40 766.90(5)	40 766.888(24)	67A	33 814.03(5)	33 814.053(25)	67A	13
14	47 023.20(8)	47 023.167(29)	67A	39 003.36(5)	39 003.348(29)	67A	14
15	53 721.78(8)	53 721.736(33)	67A	44 559.55(5)	44 559.520(34)	67A	15
16	60 861.63(8)	60 861.654(38)	67A	50 481.79(8)	50 481.793(41)	67A	16
17	...	68 441.917(42)		56 769.32(8)	56 769.344(47)	67A	17
18	76 461.43(10)	76 461.461(49)	67A	63 421.28(8)	63 421.301(52)	67A	18
19	...	84 919.164(65)		70 436.84(10)	70 436.743(57)	67A	19
20	93 813.85(10)	93 813.842(98)	67A	77 814.65(10)	77 814.703(66)	67A	20
21	...	103.144.25(15)		...	85 554.169(90)		21
22	...	112 909.10(23)		93 654.08(10)	93 654.082(139)	67A	22

<sup>a</sup>  $\nu_2$  is at 712  $\text{cm}^{-1}$  for HCN and at 569  $\text{cm}^{-1}$  for DCN.

Table 20. Hyperfine Structure for the  $\lambda$ -doublets of the  $01^1_0$  State of HCN

J	$F'_N - F''_N$	$F' - F''$	Observed Frequency (MHz)	Relative Intensity	Ref.
1	0	1	$\frac{1}{2}$	450.8211(10)	6
			$\frac{1}{2}$	450.8017(6)	10
2	1	$\frac{5}{2}$	$\frac{3}{2}$	449.6082(4)	16
		$\frac{3}{2}$	$\frac{1}{2}$	449.5938(8)	8
		$\frac{3}{2}$	$\frac{3}{2}$	449.5736(30)	2
2	2	$\frac{5}{2}$	$\frac{3}{2}$	448.9963(30)	2
		$\frac{5}{2}$	$\frac{5}{2}$	448.9627(2)	32
		$\frac{3}{2}$	$\frac{5}{2}$	448.9289(30)	2
1	1	$\frac{3}{2}$	$\frac{1}{2}$	448.8643(30)	2
		$\frac{5}{2}$	$\frac{3}{2}$	448.8449(8)	8
		$\frac{1}{2}$	$\frac{1}{2}$	448.8250(30)	2
1	2	$\frac{3}{2}$	$\frac{3}{2}$	448.2333(60)	1
		$\frac{1}{2}$	$\frac{3}{2}$	448.2131(10)	6
		$\frac{3}{2}$	$\frac{5}{2}$	448.1996(6)	10
2	2	2	-	1 346.677(10)	23
		3	3	1 346.796(10)	56
		1	1	-	
3	3	3	-	2 693.250(18)	28
		4	4	-	
		2	2	2 693.395(12)	61
3	2	2	-	2 691.757(16)	3
		3	4	-	
		4	3	2 692.071(12)	3
2	3	3	-	2 694.582(18)	3
		4	4	-	
		5	5	2 694.954(18)	3
4	4	4	-	4 488.381(40)	30
		5	5	-	
		3	3	4 488.522(40)	63
4	3	3	-	4 486.762(26)	2
		4	5	-	
		5	5	4 487.000(12)	2
5	5	5	-	6 731.793(22)	31
		6	6	-	
		4	4	6 731.925(18)	64

Table 21.  $\lambda$ -Doublet Transitions Observed for Other Isotopic Species [Ref. 61A]

Molecule	J	Observed Frequency (MHz)
$H^{13}C^{14}N$	6	9 018.87(5)
	7	12 023.25(5)
( $01^1_0$ state at $706\text{ cm}^{-1}$ )	8	15 455.64(10)
	9	19 315.70(10)
	10	23 602.60(10)
$H^{12}C^{15}N$	6	8 897.20(10)
	7	11 861.0(2)
( $01^1_0$ state at $711\text{ cm}^{-1}$ )	8	15 247.1(2)
	9	19 055.4(3)
	10	23 284.1(3)
$D^{13}C^{14}N$	6	7 652.70(5)
	7	10 201.95(5)
( $01^1_0$ state at $563\text{ cm}^{-1}$ )	8	13 114.35(10)
	9	16 389.63(10)
	10	20 027.10(10)
	11	24 026.60(10)
$D^{12}C^{15}N$	6	7 391.80(10)
	7	9 854.15(10)
( $01^1_0$ state at $568\text{ cm}^{-1}$ )	8	12 667.25(10)
	9	15 830.90(10)
	10	19 344.30(10)
	11	23 207.45(20)

Table 22. Doublet Transitions Measured for the  $030$  State of HCN and DCN

	J	Observed Frequency (MHz)	Ref.
HCN	4	9 242.20(10)	61A
( $03^1_0$ state at $2113\text{ cm}^{-1}$ )	5	13 861.45(10)	61A
	6	19 402.20(10)	61A
	7	25 863.35(10)	61A
DCN	4	7 634.45(10)	61A
( $03^1_0$ state at $1691\text{ cm}^{-1}$ )	5	11 449.55(10)	61A
	6	16 025.35(10)	61A
	7	21 360.15(10)	61A
	8	27 450.96(20)	67A
	9	34 294.02(20)	67A
	10	41 884.00(20)	67A
DCN	24	9 570.98(20)	67A
( $03^3_0$ state at $1707\text{ cm}^{-1}$ )	25	12 033.46(20)	67A
	26	14 958.90(20)	67A
	27	18 396.45(20)	67A
	28	22 392.32(20)	67A
	29	26 989.05(20)	67A
	30	32 224.05(20)	67A
	31	38 128.05(20)	67A

Table 23. *l*-Type Resonance Doublets Measured for the  $02^20$  State<sup>a</sup> of HCN and DCN [Ref. 67A]

	HCN Observed Frequency (MHz)	J	DCN Observed Frequency (MHz)
...	15	8	306.60(10)
8 292.88(10)	16	10	586.85(10)
10 464.07(10)	17	13	272.45(10)
13 019.97(10)	18	16	393.87(10)
15 995.82(10)	19	19	977.48(10)
19 426.18(10)	20	24	045.83(10)
23 343.70(15)	21	28	616.97(15)
27 778.92(15)	22	33	704.62(15)
32 759.76(15)	23	39	317.87(15)
38 311.12(15)	24	45	462.56(15)
44 454.32(15)	25	...	

<sup>a</sup>The  $02^20$  state is at  $1427\text{ cm}^{-1}$  for HCN and  $1138\text{ cm}^{-1}$  for DCN.

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