

Microwave Spectra of Molecules of Astrophysical Interest

XIII. Cyanoacetylene

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The microwave spectrum of cyanoacetylene is critically reviewed for information applicable to radio astronomy. Molecular data such as the derived rotational constants, centrifugal distortion parameters, hyperfine coupling constants, electric dipole moment and molecular structure are tabulated. The observed rotational transitions are presented for the astronomically interesting isotopic forms and low-lying vibrational states of cyanoacetylene. Calculated rotational transitions up to 300 GHz are presented for the ground vibrational state of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$, $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$, $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$, $\text{H}^{12}\text{C}^{12}\text{C}^{13}\text{C}^{14}\text{N}$, $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{15}\text{N}$, and $\text{D}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$, and for the vibrationally excited states ν_5 , ν_6 , ν_7 , $2\nu_7$, and $3\nu_7$ of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$.

Key words: Cyanoacetylene; interstellar molecules; line strengths; microwave spectra; molecular constants; radio astronomy; rotational transitions.

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1. Introduction

The present work is part of a series of critical reviews which are intended to update, revise, and augment the existing literature on molecules which have been identified in interstellar molecular clouds. In order to provide complete coverage of the spectral regions where present and anti-

ipated radio telescope receivers operate, all measured and predicted rotational transitions are included up to 300 GHz. For the ℓ -doubling lines of the vibrationally excited states, the predicted transitions were limited to rotational levels up to $J=60$ for the ν_5^1 state, $J=50$ for the $3\nu_7^1$ state, $J=28$ for the ν_6^1 state and $J=25$ for the ν_7^1 state.

Since cyanoacetylene was first detected in interstellar molecular clouds by B. E. Turner in 1970 [1]¹, numerous rotational lines of the normal isotopic form, $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$, have been observed toward several astronomical sources.

¹ Numbers in brackets indicate literature references in section 2.5.

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Quite recently transitions from all three ^{13}C isotopic forms have been observed and several millimeter wavelength transitions from the ν_7^1 vibrational state have been reported. Because of these reported observations the rotational spectra of the singly substituted isotopic forms of cyanoacetylene, i.e., $\text{H}^{13}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$, $\text{H}^{12}\text{C}^{13}\text{C}^{12}\text{C}^{14}\text{N}$, $\text{H}^{12}\text{C}^{12}\text{C}^{13}\text{C}^{14}\text{N}$, $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{15}\text{N}$, and $\text{D}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$, as well as the spectra of the low energy vibrational states ν_5 , ν_6 , ν_7 , $2\nu_7$ and $3\nu_7$ of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ are included in this review in order to thoroughly cover the species observed and those which might be observed with improved astronomical instrumentation.

2. Organization of the Spectral Tables

The molecular constants for all isotopic forms and vibrational states of cyanoacetylene considered in this work are given in table 1. The microwave spectral transitions of each of the cyanoacetylene species and vibrational states are given separately in table 2 through table 13. Table 14 contains a list of all the calculated transitions reported here, ignoring hyperfine splittings, ordered by increasing frequency as an aid to the user.

The open literature relating to laboratory and astronomical studies of HCCCN has been searched through June 1977. All pertinent references are given in section 3.1.

2.1. Molecular Parameter Tables

The rotational and centrifugal distortion constants for $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$, $\text{D}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$, $\text{H}^{13}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$, $\text{H}^{12}\text{C}^{13}\text{C}^{12}\text{C}^{14}\text{N}$, $\text{H}^{12}\text{C}^{12}\text{C}^{13}\text{C}^{14}\text{N}$, and $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{15}\text{N}$ are given in table 1. Also found in table 1 are the quadrupole coupling constants, $(eqQ)_v$, and, in one case, where the available data are very precise, the spin-rotation interaction constant, $C_r(N^{14})$, both of which arise from the nitrogen nucleus with spin equal 1, the dipole moment of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ and the molecular structure.

a. Parameters for the Ground State

The spectroscopic constants of the ground states of the various isotopic species were derived using the following expression for the energy of a Σ state rotational level with given values of the quantum numbers J and F :

$$F_v(J) = B_v J(J+1) - D_v J^2(J+1)^2 + H_v J^3(J+1)^3 + (eqQ)_v \left[\frac{3/4 C(C+1) - 2J(J+1)}{2(2J-1)(2J+3)} \right] + 1/2 C_r(N^{14}) [F(F+1) - 2 - J(J+1)] \quad (1)$$

where $J=0,1,2,\dots$; $F=J+1, J, J-1$; and $C=F(F+1) - 2 - J(J+1)$. The last two terms in equation 1 are required, of course, only when a ^{14}N nucleus is present in the molecule. A weighted least-squares fitting of all observed transitions including hyperfine components was simultaneously carried out following closely the procedures suggested by Kirchhoff [2]. Each datum was assigned a weight equal to the reciprocal of the

square of its estimated uncertainty; blended lines were assigned zero weighting in the fitting. In the case of $\text{D}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ where insufficient data exist to determine the quadrupole coupling constant $(eqQ)_v$, the value of this constant determined for $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ was used to estimate the center frequency of the low J transitions from the unblended hyperfine components that were observed.

b. Parameters for Excited Vibrational States

The three lowest fundamental vibrations of the cyanoacetylene molecule are skeletal bending modes. These vibrations are doubly degenerate having Π vibrational symmetry. This degeneracy is split by rotation into a pair of levels designated by convention as e or f levels. In this case the lower of the levels is an e state; the higher, f . The rotational energy of a Π state is given by:

$$F_v(J) = (B_v \pm 1/2 q_v) J(J+1) - D_v [J(J+1) - 1]^2 + (eqQ)_v \left[\frac{3}{J(J+1)} - 1 \right] \left[\frac{3/4 C(C+1) - 2J(J+1)}{2(2J-1)(2J+3)} \right] \quad (2)$$

where $q_v = q_v^0 + q_v^1 J(J+1)$, $J=1,2,3,\dots$, and F and C have been defined above. The plus sign applies to f levels; the minus sign to e levels. Both $\Delta J=+1$ and $\Delta J=0$ transitions have been observed for the ν_7^1 vibrational state, and both of these type transitions have been simultaneously fit to obtain the spectroscopic constants of this state.

Constants are also tabulated for two overtone levels of the ν_7 vibration. The rotational energy level expressions for these levels are complicated by l -type resonances, i.e. interactions between the various l components of an overtone. Maki and Lide [3] have derived equations to account for this resonance in the HCN molecule. Somewhat simpler expressions have proven to be adequate to treat l -type resonance in cyanoacetylene; the following expressions have been deduced from those given in reference [3].

For the $2\nu_7^2$ (Σ) and $2\nu_7^2$ (Δ) levels the following expressions apply:

for $l=0$

$$F_v(J) = B_v J(J+1) - D_v J^2(J+1)^2 - \frac{q_v^2}{\Delta_{02}} [J^2(J+1)^2 - 2J(J+1)] - (eqQ)_v \left[\frac{3/4 C(C+1) - 2J(J+1)}{2(2J-1)(2J+3)} \right] \quad (3)$$

$l=2$ (e levels)

$$F_v(J) = B_v J(J+1) - D_v [J(J+1) - 4]^2 + 4\gamma_{ll} J(J+1) + (eqQ)_v \left[\frac{12}{J(J+1)} - 1 \right] \left[\frac{3/4 C(C+1) - 2J(J+1)}{2(2J-1)(2J+3)} \right] \quad (4)$$

and, for $l=2$ (f levels),

$$F_v(J) = B_v J(J+1) - D_v [J(J+1) - 4]^2 + 4\gamma_{ll} J(J+1) + \frac{q_v^2}{\Delta_{02}} [J^2(J+1)^2 - 2J(J+1)] + (eqQ)_v \left[\frac{12}{J(J+1)} - 1 \right] \left[\frac{3/4 C(C+1) - 2J(J+1)}{2(2J-1)(2J+3)} \right] \quad (5)$$

where Δ_{02} is the vibrational energy difference between the $l=0$ and $l=2$ states. γ_{ll} is a small term which corrects for the l -dependence of the B rotational constant and $J=0, 1, 2, 3 \dots$ for the $l=0$ states and $J=2, 3, 4 \dots$ for the $l=2$ states. All data for the $2\nu_7$ states have been fit simultaneously.

In addition to l -type resonance the energy levels of the $3\nu_7^2$ (Π) and $3\nu_7^2$ (Φ) states appear to be further complicated by an accidental vibrational resonance. Using the vibrational and anharmonic constants of Mallinson and Fayt [4], the $3\nu_7^2$ vibrational level is found to fall at 664.7 cm^{-1} ; the $3\nu_7^2$ levels at 663.3 cm^{-1} . The vibrational frequency of the ν_7^2 vibration is 663.21 cm^{-1} . The effect of this higher-order resonance is to introduce very small but significant discrepancies between the constants determined for the $l=1$ and $l=3$ levels. Because of this the $l=1$ and $l=3$ levels have been fit separately and empirically. The rotational energy of the $3\nu_7^2$ state has been taken for the e levels as:

$$F(J) = B_v^* J(J+1) - D_v^* [J(J+1) - 1]^2 + 1/2 \Delta_{13} - 1/2 W_{11} - 1/2 [(\Delta_{13} + W_{11})^2 + 4W_{31}^2]^{1/2} + (eqQ)_v \left[\frac{3}{J(J+1)} - 1 \right] \left[\frac{3/4 C(C+1) - 2J(J+1)}{2(2J-1)(2J+3)} \right] \quad (6)$$

and for the f levels:

$$F(J) = B_v^* J(J+1) - D_v^* [J(J+1) - 1]^2 + 1/2 \Delta_{13} + 1/2 W_{11} - 1/2 [(\Delta_{13} - W_{11})^2 + 4W_{31}^2]^{1/2} + (eqQ)_v \left[\frac{3}{J(J+1)} - 1 \right] \left[\frac{3/4 C(C+1) - 2J(J+1)}{2(2J-1)(2J+3)} \right] \quad (7)$$

where $J=1, 2, 3, \dots$; Δ_{13} is the vibrational energy difference between the $l=1$ and $l=3$ levels, $W_{11} = q_v J(J+1)$, $W_{31} = \sqrt{3/2} q_v [J^2(J+1)^2 - 8J(J+1) + 12]^{1/2}$, q_v has been defined above, and the superscript asterisk indicates effective constants.

The $3\nu_7^2$ rotational levels will be split by l -type resonance. In this work to the highest J transition observed, however, no splitting was apparent. The following rotational energy level expression was, therefore, found to be adequate to the limit of the observations:

$$F_v(J) = B_v^* J(J+1) - D_v^* [J(J+1) - 9]^2 + eqQ \left[\frac{27}{J(J+1)} - 1 \right] \left[\frac{3/4 C(C+1) - 2J(J+1)}{2(2J-1)(2J+3)} \right] \quad (8)$$

where $J=3, 4, 5, \dots$

Insufficient unblended data for the determination of the quadrupole coupling constant, $(eqQ)_v$, was available from the vibrational state rotational lines. The value of this constant determined for the ground state of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ was used to estimate the center frequency of the low J transitions from the unblended hyperfine components that were observed, and these frequencies were included in the least-squares fitting.

Transitions used in the fitting are for the most part taken from previously reported measurements. In a few cases, however, where significant improvement would result in the derived constants, selected lines were measured in this laboratory on a conventional Stark modulated spectrometer. The dipole moment reported was measured in this laboratory using a high precision dc voltage supply superimposed with just sufficient voltage from a 80 kHz square-wave generator to modulate the Stark split lines. The guide spacing was calibrated with OCS using the dipole moment of Müenter [5].

2.2. Microwave Spectral Tables

The results of the statistical analysis of the rotational spectrum of the various isotopic species of cyanoacetylene and the lower-lying vibrational states of the most abundant isotopic species are given in tables 2 through 13. The frequencies included in these tables include all transitions with sufficient intensity over the range 5–300,000 MHz. The first column gives the upper and lower state rotational quantum numbers of the transition in question. If vibrational angular momentum exists for the vibrational state in question, the l quantum numbers are also included. The observed unsplit line frequency follows next. In many of the lower J transitions, where the hyperfine splittings are only incompletely resolved, an estimate of the center frequency has been calculated from the unblended hyperfine components using the value of $(eqQ)_v$ determined for the ground state of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$. The calculated frequencies and statistical uncertainty (one standard deviation) follow in the next column. For transitions with J less than 9, the observed and calculated hyperfine components of the transition in question is listed underneath each center frequency. The hyperfine components were limited to those with relative intensities ≥ 0.01 for each rotational transition. In those cases where it has been necessary for lack of data to assume a value of $(eqQ)_v$, a footnote in the table indicates that this has been done and no uncertainties are given for the frequencies of the hyperfine components so calculated.

The expression for the line strengths of linear molecules are particularly simple. For $\Delta J = +1$ transitions

$$S(J, J') = \frac{J''+1)^2 - l^2}{(J''+1)}, \quad (9)$$

while for $J=0$ transitions

$$S(J, J) = \frac{(2J+1)l^2}{J(J+1)}. \quad (10)$$

Values of the line strength of each transition are also included in the table. For those transitions where the frequencies of the quadrupole hyperfine components are given, the line strength of each separate component is also included.

The energy of the lowest level in a ground state transition has been calculated from the constants obtained in this work. For the vibrational state, vibrational energy levels calculated from the vibrational and anharmonic constants of Mallinson and Fayt [4] have been used in addition to the rotational constants of this work.

For the convenience of the user, the center frequencies of all transitions calculated in this work are arranged in numerical order in table 14.

2.3. Corrections and Comments on the Laboratory and Astronomical Literature

One of the primary objectives of this work is to provide accurate transition frequencies for astronomical studies. Since many astronomical studies of cyanoacetylene have been reported prior to this work, several comments regarding corrections to the prior laboratory and astronomical literature are necessary.

During the reanalysis of the v_7^1 state of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$, we found that the measurements of the $J=10-9$, $l=1f$ transition reported by Tyler and Sheridan [5] deviated substantially from the calculated value. Remeasurement of the $J=10-9$ transitions, as listed in table 8, provided an improved value compared to the earlier work. This transition has also been detected in the Orion A molecular cloud [6] and the cloud velocity derived was based on the frequency given by Tyler and Sheridan. From the more accurate calculated frequency of this transition the corrected velocity for this observation is 6.6 km s^{-1} , which is consistent with that determined by Clark et al. [6] for the lower frequency l -component of the $J=10-9$ transition.

A second objective of reviews of this type is to provide spectral data useful for identifying interstellar molecular lines attributable to known interstellar species. After completing this review, we noted that one of the unidentified lines reported by B. E. Turner [7] toward the Sagittarius B2 molecular cloud appears to be assignable to ^{13}C isotopes of cyanoacetylene. The frequency of the unidentified line is given as 81542.7 MHz (see fig. 1(d) in [7]) which agrees quite well with the $J=9-8$ transition of $\text{H}^{12}\text{C}^{12}\text{C}^{13}\text{C}^{14}\text{N}$ calculated at 81541.9815(98) MHz. The $J=9-8$ transition of $\text{H}^{12}\text{C}^{13}\text{C}^{12}\text{C}^{14}\text{N}$ at 81534.125(11) MHz also lies within the observed width of the observation reported by Turner.

2.4. List of Symbols

B_v	Rotational constant for the ground ($v=0$) or excited state ($v \neq 0$).
D_v, H_v	Quartic and sextic centrifugal distortion constants for v^{th} state.
$(e q Q)_v$	Nuclear electric quadrupole coupling constant for v^{th} state.
C_x	Spin-rotation hyperfine coupling constant related to nucleus X.
q_v	l -doubling constant.
μ	Electric dipole moment.
Δ_{02}	Vibrational energy difference between the $l=0$ and $l=2$ levels of $2\nu_7$.
Δ_{13}	Vibrational energy difference between the $l=1$ and $l=3$ levels of $3\nu_7$.
γ_{ll}	Higher-order rotational constants which correct the B_v values of a given rotational level for the effects of vibrational angular momentum.
J	Total rotational angular momentum quantum number.
F	Total angular momentum quantum number which includes nuclear spin.
$v-\nu_n^l$	Vibrational mode for v^{th} state of the n^{th} vibration and l^{th} vibrational angular momentum.
l	Quantum number for vibrational angular momentum.
(...)	Parentheses in the numerical listings contain measured uncertainties or standard deviations for calculated quantities.

2.5. References

- [1] B. E. Turner, *Astrophys. J. (Letters)* **163**, L35 (1971). "Detection of Interstellar Cyanoacetylene."
- [2] W. H. Kirchhoff, *J. Mol. Spectrosc.* **41**, 333 (1972). "On the Calculation of Centrifugal Distortion Constants: A Statistical Basis for Model Testing: The Calculation of the Force Field."
- [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 Resonance Doublets."
- [4] P. D. Mallinson and A. Fayt, *Mol. Phys.* **32**, 473 (1976). "High Resolution Infrared Studies of HCCCN and DCCCN."
- [5] J. S. Muentzer, *J. Chem. Phys.* **48**, 4544 (1968). "Electric Dipole Moment of Carbonyl Sulfide."
- [6] F. O. Clark, R. D. Brown, P. D. Godfrey, J. W. V. Storey and D. R. Johnson, *Astrophys. J. (Letters)* **210**, L139 (1976). "Detection of Interstellar Vibrationally Excited Cyanoacetylene."
- [7] B. E. Turner, *Astrophys. J. (Letters)* **213**, L75 (1977). "Microwave Detection of Interstellar Ketene."

2.6. Acknowledgments

The authors gratefully acknowledge Drs. P. D. Mallinson and R. L. DeZafra, and Drs. R. A. Creswell, G. Winnewisser, and M. C. L. Gerry for communicating pre-publication copies of their laboratory studies on cyanoacetylene.

3. Cyanoacetylene Spectral Tables

Table 1. Molecular Constants of Cyanoacetylene.

Molecule	Ground State Constants				
	B_0 (MHz)	D_0 (kHz)	H_0 (nHz)	$eqQ(^{14}N)$ (kHz)	$C_T(^{14}N)$ (kHz)
$H^{12}C^{12}C^{12}C^{14}N$	4549.05896(14) ^a	0.54695(82) ^a	3.5(16) ^a	-4318.8(12) ^a	1.05(26) ^a
$H^{12}C^{12}C^{13}C^{14}N$	4530.19760(46)	0.5401(21)	-0.84(242)	-4300.1(67)	----
$H^{12}C^{13}C^{12}C^{14}N$	4529.7617(13)	0.5438(62)	0.58(896)	-4298.(23)	----
$H^{13}C^{12}C^{12}C^{14}N$	4408.4423(11)	0.5088(56)	-2.8(85)	-4273.(19)	----
$H^{12}C^{12}C^{12}C^{15}N$	4416.75278(98)	0.5099(49)	-3.4(72)	----	----
$D^{12}C^{12}C^{12}C^{14}N$	4221.58167(44)	0.4530(18)	1.1(16)	-4318.8 ^b	----

State	Vibrational State Constants of $H^{12}C^{12}C^{12}C^{14}N$		
	B_V (MHz)	D_V (kHz)	q_V (MHz)
v_5^1	4550.7777(40)	0.732(16)	2.5811(80) - 8.0(32) × 10 ⁻⁵ J(J+1)
v_6^1	4558.3064(21)	0.5399(91)	3.5886(43) - 4.1(18) × 10 ⁻⁵ J(J+1)
v_7^1 ^d	4563.5105(17)	0.5688(20)	6.538254(33) - 1.5983(12) × 10 ⁻⁵ J(J+1)
$2v_7^{0,2}$	4577.9708(28)	0.5984(31)	c
$3v_7^1$ ^e	4592.1931(43)	0.334(22)	6.58153(18) - 1.134(26) × 10 ⁻⁵ J(J+1)
$3v_7^3$	4592.2606(34)	0.392(14)	----

Dipole Moment ($H^{12}C^{12}C^{12}C^{14}N$)

$$\mu = 3.724(30) \text{ D}$$

Molecular Structure^f

Bond	Bond Distance (Å)
H-C	1.057
C≡C	1.205
C-C	1.378
C≡N	1.159

^a The numbers in parenthesis are standard errors in units of the last significant figures.

^b Fixed at value determined for $H^{12}C^{12}C^{12}C^{14}N$.

^c $q^2/\Delta_{02} = 0.6314(27) \text{ kHz}$; $\gamma_{\ell\ell} = -14.82(84) \text{ kHz}$.

^d $(eqQ)_V = 4266(63) \text{ kHz}$.

^e $\Delta_{13} = 4.245(15) \text{ cm}^{-1}$.

^f Structure derived in Reference [58A] with data from Reference [50A]. The bond distances reported are r_s distances.

Table 2. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the Ground State.

Transition $J'-J''$	$F'-F''$	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
1- 0			9 098.1157(3)	1.000	0.00	
	1- 1	9 097.0346(3)	9 097.0350(5)	0.333		71A
	2- 1	9 098.3321(3)	9 098.3327(4)	0.555		71A
	0- 1	9 100.2727(5)	9 100.2730(8)	0.111		71A
2- 1			18 196.2183(5)	2.000	0.30	
	2- 2	18 194.936(20)	18 194.9206(8)	0.167		77A
	1- 0	18 195.190(50)	18 195.3176(6)	0.222		77A
	2- 1	18 196.279(50)*	18 196.2183(5)	0.500		77A
	3- 2		18 196.3119(7)	0.932		
	1- 2		18 197.0779(11)	0.011		
	1- 1	18 198.366(20)	18 198.3756(9)	0.167		77A
3- 2			27 294.2947(8)	3.000	0.91	
	3- 3	27 292.904(10)	27 292.9033(11)	0.111		77A
	2- 1	27 294.065(30)	27 294.0777(8)	0.600		77A
	3- 2	27 294.314(30)*	27 294.2947(8)	0.888		77A
	4- 3		27 294.3471(9)	1.287		
	2- 2	27 296.230(10)	27 296.2349(11)	0.111		77A
4- 3			36 392.3316(10)	4.000	1.82	
	4- 4	36 390.892(10)	36 390.8878(13)	0.083		77A
	3- 2	36 392.326(100)*	36 392.2380(10)	0.952		77A
	4- 3		36 392.3316(10)	1.252		
	5- 4		36 392.3654(11)	1.628		
	3- 3	36 394.169(10)	36 394.1783(14)	0.083		77A
5- 4			45 490.3161(12)	5.000	3.03	
	5- 5		45 488.8386(16)	0.067		
	4- 3		45 490.2637(12)	1.295		
	5- 4		45 490.3161(12)	1.600		
	6- 5		45 490.3399(13)	1.970		
	4- 4		45 492.1104(16)	0.067		
6- 5		54 588.247(5)	54 588.2351(14)	6.000	4.55	71A
	6- 6		54 586.7338(19)	0.056		
	5- 4		54 588.2013(13)	1.638		
	6- 5		54 588.2351(14)	1.944		
	7- 6		54 588.2527(15)	2.310		
	5- 5		54 589.9955(19)	0.056		
7- 6		63 686.052(10)	63 686.0753(15)	7.000	6.37	71A
	7- 7		63 684.5563(22)	0.048		
	6- 5		63 686.0516(15)	1.974		
	7- 6		63 686.0753(15)	2.289		
	8- 7		63 686.0891(16)	2.646		
	6- 6		63 687.8120(22)	0.048		

Table 2. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the Ground State (Continued).

Transition J'-J''	F'-F''	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
8-7		72 783.822(15)	72 783.8238(17)	8.000	8.50	71A
	8-8		72 782.2911(25)	0.042		
	7-6		72 783.8061(17)	2.312		
	8-7		72 783.8238(17)	2.624		
	9-8		72 783.8349(18)	2.984		
	7-7		72 785.5429(25)	0.042		
9-8			81 881.4675(19)	9.000	10.93	
10-9		90 979.023(20)	90 978.9933(21)	10.000	13.66	77A
11-10		100 076.392(15)	100 076.3883(23)	11.000	16.69	71A
12-11		109 173.634(4)	109 173.6394(25)	12.000	20.03	71A
13-12		118 270.68(20)	118 270.7336(26)	13.000	23.67	77C
14-13		127 367.666(50)	127 367.6581(25)	14.000	27.62	77A
15-14			136 464.3999(23)	15.000	31.86	
16-15		145 560.946(30)	145 560.9462(19)	16.000	36.42	
17-16		154 657.284(1)	154 657.2840(16)	17.000	41.27	71A
18-17		163 753.389(15)	163 753.4007(24)	18.000	46.43	71A
19-18		172 849.300(40)	172 849.2834(47)	19.000	51.89	77A
20-19		181 944.923(40)	181 944.9194(81)	20.000	57.66	77A
21-20		191 040.299(50)	191 040.296(13)	21.000	63.73	77A
22-21		200 135.392(22)	200 135.401(19)	22.000	70.10	71A
23-22		209 230.234(3)	209 230.221(26)	23.000	76.78	77A
24-23		218 324.788(50)	218 324.744(36)	24.000	83.76	77A
25-24			227 418.957(47)	25.000	91.04	
26-25			236 512.849(62)	26.000	98.62	
27-26			245 606.406(79)	27.000	106.51	
28-27			254 699.617(99)	28.000	114.71	
29-28			263 792.47(12)	29.000	123.20	
30-29			272 884.95(15)	30.000	132.00	
31-30			281 977.05(18)	31.000	141.10	
32-31			291 068.75(22)	32.000	150.51	
33-32			300 160.05(26)	33.000	160.22	

* Blended lines not included in least-squares fitting.

Table 3. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{13}\text{C}^{14}\text{N}$ in the Ground State.

Transition $J'-J''$	$F'-F''$	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
1- 0			9 060.3930(9)	1.000	0.00	
	1- 1	9 059.330(10)	9 059.3180(20)	0.333		77A
	2- 1	9 060.617(10)	9 060.6080(9)	0.555		77A
	0- 1	9 062.553(10)	9 062.5431(34)	0.111		77A
2- 1			18 120.7731(18)	2.000	0.30	
	2- 2	18 119.497(20)	18 119.4831(29)	0.167		77A
	1- 0	18 119.750(50)	18 119.6981(26)	0.222		77A
	2- 1	18 120.826(50)*	18 120.7731(18)	0.500		77A
	3- 2		18 120.8653(18)	0.932		
	1- 2		18 121.6331(21)	0.011		
	1- 1	18 122.918(20)	18 122.9232(36)	0.167		77A
3- 2			27 181.1273(26)	3.000	0.91	
	3- 3	27 179.745(10)	27 179.7451(36)	0.111		77A
	2- 1	27 180.885(30)	27 180.9123(27)	0.600		77A
	3- 2	27 181.151(30)*	27 181.1273(26)	0.888		77A
	4- 3		27 181.1785(26)	1.287		
	2- 2	27 183.064(10)	27 183.0623(37)	0.111		77A
4- 3			36 241.4425(33)	4.000	1.81	
	4- 4	36 240.007(10)	36 240.0092(42)	0.085		77A
	3- 2	36 241.435(100)*	36 241.3504(33)	0.952		77A
	4- 3		36 241.4425(33)	1.252		
	5- 4		36 241.4751(33)	1.628		
	3- 3	36 243.281(10)	36 243.2854(41)	0.083		77A
5- 4			45 301.7059(39)	5.000	3.02	
	5- 5		45 300.2400(48)	0.067		
	4- 3		45 301.6547(39)	1.295		
	5- 4		45 301.7059(39)	1.600		
	6- 5		45 301.7285(39)	1.970		
	4- 4		45 303.4976(45)	0.067		
6- 5			54 361.9045(44)	6.000	4.53	
	6- 6		54 360.4160(52)	0.056		
	5- 4		54 361.8719(44)	1.638		
	6- 5		54 361.9045(44)	1.944		
	7- 6		54 361.9210(44)	2.310		
	5- 5		54 363.6636(48)	0.056		
7- 6			63 422.0253(48)	7.000	6.35	
	7- 7		63 420.5203(56)	0.048		
	6- 5		63 422.0027(48)	1.974		
	7- 6		63 422.0253(48)	2.289		
	8- 7		63 422.0379(48)	2.646		
	6- 6		63 423.7618(52)	0.048		

Table 3. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{13}\text{C}^{14}\text{N}$ in the Ground State (Continued).

Transition $J'-J''$ $F'-F''$	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
8- 7		72 482.0553(51)	8.000	8.46	
	8- 8	72 480.5376(59)	0.042		
	7- 6	72 482.0387(51)	2.312		
	8- 7	72 482.0553(51)	2.624		
	9- 8	72 482.0652(51)	2.984		
	7- 7	72 483.7753(54)	0.042		
9- 8		81 541.9815(54)	9.000	10.88	
10- 9	90 601.777(25)	90 601.7910(58)	10.000	13.60	77A
11-10		99 661.4707(64)	11.000	16.62	
12-11	108 720.999(35)	108 721.0077(72)	12.000	19.95	77A
13-12	117 780.398(30)	117 780.3890(81)	13.000	23.57	77A
14-13		126 839.6015(92)	14.000	27.50	
15-14		135 898.632(10)	15.000	31.73	
16-15	144 957.486(40)	144 957.468(11)	16.000	36.27	77A
17-16	154 016.091(40)	154 016.096(12)	17.000	41.10	77A
18-17		163 074.504(13)	18.000	46.24	
19-18	172 132.670(40)	172 132.677(14)	19.000	51.68	77A
20-19	181 190.614(50)	181 190.603(14)	20.000	57.42	77A
21-20		190 248.270(16)	21.000	63.46	
22-21		199 305.663(18)	22.000	69.81	
23-22		208 362.770(24)	23.000	76.46	
24-23	217 419.574(50)	217 419.577(32)	24.000	83.41	77A
25-24		226 476.072(44)	25.000	90.66	
26-25		235 532.241(59)	26.000	98.21	
27-26		244 588.071(79)	27.000	106.07	
28-27		253 643.55(10)	28.000	114.23	
29-28		262 698.66(13)	29.000	122.69	
30-29		271 753.40(17)	30.000	131.45	
31-30		280 807.74(21)	31.000	140.52	
32-31		289 861.68(26)	32.000	149.88	
33-32		298 915.20(31)	33.000	159.55	

* Blended lines not included in least-squares fitting.

Table 4. Rotational Spectrum of $\text{H}^{12}\text{C}^{13}\text{C}^{12}\text{C}^{14}\text{N}$ in the Ground State.

Transition $J'-J''$	$F'-F''$	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
1- 0			9 059.5212(25)	1.000	0.00	
	1- 1	9 058.498(30)	9 058.4468(60)	0.333		76A
	2- 1	9 059.739(50)	9 059.7361(28)	0.555		76A
	0- 1	9 061.700(50)	9 061.6700(119)	0.111		76A
2- 1			18 119.0294(48)	2.000	0.30	
	2- 2 } 1- 0 }	18 117.774(100)*	18 117.7401(80) 18 117.9550(71)	0.167 0.222		77A
	2- 1 } 3- 2 }	18 119.098(50)*	18 119.0294(48) 18 119.1215(49)	0.500 0.932		77A
	1- 2		18 119.8889(70)	0.011		
	1- 1		18 121.1782(128)	0.167		
3- 2			27 178.5115(69)	3.000	0.91	
	3- 3	27 177.129(20)	27 177.1301(96)	0.111		77A
	2- 1	27 178.266(40)	27 178.2966(69)	0.600		77A
	3- 2 } 4- 3 }	27 178.530(30)*	27 178.5115(69) 27 178.5626(70)	0.888 1.287		77A
	2- 2	27 180.446(20)	27 180.4454(129)	0.111		77A
4- 3			36 237.9544(87)	4.000	1.81	
	4- 4	36 236.516(20)	36 236.5218(110)	0.083		77A
	3- 2 } 4- 3 } 5- 4 }	36 237.945(100)*	36 237.8623(87) 36 237.9544(87) 36 237.9869(87)	0.952 1.252 1.628		77A
	3- 3	36 239.779(40)	36 239.7962(137)	0.083		77A
5- 4			45 297.345(10)	5.000	3.02	
	5- 5		45 295.880(12)	0.067		
	4- 3		45 297.294(10)	1.295		
	5- 4		45 297.345(10)	1.000		
	6- 5		45 297.368(10)	1.970		
	4- 4		45 299.136(15)	0.067		
6- 5			54 356.671(11)	6.000	4.53	
	6- 6		54 355.183(13)	0.056		
	5- 4		54 356.638(11)	1.638		
	6- 5		54 356.671(11)	1.944		
	7- 6		54 356.687(11)	2.310		
	5- 5		54 358.429(15)	0.056		
7- 6			63 415.918(11)	7.000	6.35	
	7- 7		63 414.414(13)	0.048		
	6- 5		63 415.895(11)	1.974		
	7- 6		63 415.918(11)	2.289		
	8- 7		63 415.930(11)	2.646		
	6- 6		63 417.653(15)	0.048		

Table 4. Rotational Spectrum of $\text{H}^{12}\text{C}^{13}\text{C}^{12}\text{C}^{14}\text{N}$ in the Ground State (Continued).

Transition $J'-J''$	$F'-F''$	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
8-7			72 475.074(11)	8.000	8.46	
	8-8		72 473.557(13)	0.042		
	7-6		72 475.057(11)	2.312		
	8-7		72 475.074(11)	2.624		
	9-8		72 475.084(11)	2.984		
	7-7		72 476.793(15)	0.042		
9-8			81 534.125(11)	9.000	10.88	
10-9		90 593.059(25)	90 593.059(11)	10.000	13.60	77A
11-10			99 651.863(12)	11.000	16.62	
12-11		108 710.532(40)	108 710.523(12)	12.000	19.94	77A
13-12		117 769.025(30)	117 769.027(14)	13.000	23.57	77A
14-13			126 827.361(15)	14.000	27.50	
15-14			135 885.513(16)	15.000	31.73	
16-15		144 943.478(40)	144 943.469(16)	16.000	36.26	77A
17-16		154 001.230(35)	154 001.217(16)	17.000	41.10	77A
18-17			163 058.743(16)	18.000	46.23	
19-18		172 115.974(40)	172 116.035(19)	19.000	51.67	77A
20-19		181 173.124(45)	181 173.079(29)	20.000	57.41	77A
21-20			190 229.863(47)	21.000	63.46	
22-21			199 286.373(72)	22.000	69.80	
23-22			208 342.60(11)	23.000	76.45	
24-23			217 398.52(15)	24.000	83.40	
25-24			226 454.13(21)	25.000	90.65	
26-25			235 509.42(27)	26.000	98.21	
27-26			244 564.37(36)	27.000	106.06	
28-27			253 618.97(46)	28.000	114.22	
29-28			262 673.20(58)	29.000	122.68	
30-29			271 727.06(72)	30.000	131.44	
31-30			280 780.53(89)	31.000	140.50	
32-31			289 833.6(11)	32.000	149.87	
33-32			298 886.2(13)	33.000	159.54	

* Blended lines not included in least-squares fitting.

Table 5. Rotational Spectrum of $\text{H}^{13}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the Ground State.

Transition J'-J''	F'-F''	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
1- 0			8 816.8825(21)	1.000	0.000	
	1- 1	8 815.824(40)	8 815.8142(57)	0.333		76A
	2- 1	8 817.115(20)	8 817.0961(21)	0.555		76A
	0- 1	8 819.065(50)	8 819.0190(91)	0.111		76A
2- 1			17 633.7527(41)	2.000	0.29	
	2- 2	17 632.56(100)*	17 632.4708(79)	0.167		77A
	1- 0		17 632.6845(71)	0.222		
	2- 1	17 633.80(50)*	17 633.7527(41)	0.500		77A
	3- 2		17 633.8443(40)	0.932		
	1- 2		17 634.6073(47)	0.011		
	1- 1	17 635.90(50)	17 635.8892(91)	0.167		77A
3- 2			26 450.5985(59)	3.000	0.88	
	3- 3	26 449.230(20)	26 449.2251(96)	0.111		77A
	2- 1	26 450.370(40)	26 450.3849(62)	0.600		77A
	3- 2	26 450.596(30)*	26 450.5985(59)	0.888		77A
	4- 3		26 450.6494(58)	1.287		
	2- 2	26 452.507(20)	26 452.5214(88)	0.111		77A
4- 3			35 267.4077(73)	4.000	1.76	
	4- 4	35 265.972(20)	35 265.9834(110)	0.083		77A
	3- 2	35 267.403(100)	35 267.3162(75)	0.952		77A
	4- 3		35 267.4077(73)	1.252		
	5- 4		35 267.4401(73)	1.628		
	3- 3	35 269.236(20)	35 269.2390(92)	0.083		77A
5- 4			44 084.1680(84)	5.000	2.94	
	5- 5		44 082.7113(120)	0.067		
	4- 3		44 084.1172(85)	1.295		
	5- 4		44 084.1680(84)	1.600		
	6- 5		44 084.1904(84)	1.970		
	4- 4		44 085.9484(97)	0.067		
6- 5			52 900.8672(90)	6.000	4.41	
	6- 6		52 899.3881(126)	0.056		
	5- 4		52 900.8349(91)	1.638		
	6- 5		52 900.8672(90)	1.944		
	7- 6		59 900.8837(90)	2.310		
	5- 5		52 902.6153(101)	0.056		
7- 6			61 717.4931(93)	7.000	6.18	
	7- 7		61 715.9976(128)	0.048		
	6- 5		61 717.4707(93)	1.974		
	7- 6		61 717.4931(93)	2.289		
	8- 7		61 717.5057(93)	2.646		
	6- 6		61 719.2187(103)	0.048		

Table 5. Rotational Spectrum of $\text{H}^{13}\text{C}^{12}\text{C}^{14}\text{N}$ in the Ground State. (Continued)

Transition J'-J''	F'-F''	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
8-7			70 534.0334(92)	8.000	8.23	
	8-8		70 532.5252(127)	0.042		
	7-6		70 534.0169(93)	2.312		
	8-7		70 534.0334(92)	2.624		
	9-8		70 534.0433(92)	2.984		
	7-7		70 535.7426(103)	0.042		
9-8			79 350.4757(90)	9.000	10.59	
10-9		88 166.832(25)	88 166.8080(89)	10.000	13.23	77A
11-10			96 983.0177(92)	11.000	16.18	
12-11		105 799.113(30)	105 799.093(10)	12.000	19.41	77A
13-12		114 614.995(30)	114 615.021(12)	13.000	22.94	77A
14-13			123 430.789(13)	14.000	26.76	
15-14			132 246.385(14)	15.000	30.88	
16-15		141 061.776(55)	141 061.797(15)	16.000	35.29	77A
17-16		149 877.008(40)	149 877.013(16)	17.000	40.00	77A
18-17			158 692.019(19)	18.000	45.00	
19-18			167 506.803(26)	19.000	50.29	
20-19		176 321.367(60)	176 321.353(38)	20.000	55.88	77A
21-20			185 135.656(56)	21.000	61.76	
22-21			193 949.699(82)	22.000	67.93	
23-22			202 763.47(12)	23.000	74.40	
24-23			211 576.96(16)	24.000	81.17	
25-24			220 390.14(21)	25.000	88.22	
26-25			229 203.02(28)	26.000	95.58	
27-26			238 015.57(36)	27.000	103.22	
28-27			246 827.79(46)	28.000	111.16	
29-28			255 639.66(58)	29.000	119.39	
30-29			264 451.17(72)	30.000	127.92	
31-30			273 262.30(88)	31.000	136.74	
32-31			282 073.0(11)	32.000	145.86	
33-32			290 883.4(13)	33.000	155.27	

* Blended lines not included in least-squares fitting.

Table 6. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{15}\text{N}$ in the Ground State.

Transition J'-J''	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
1-0	8 833.545(40)	8 833.5035(19)	1.000	0.00	77A
2-1	17 667.000(40)	17 666.9948(38)	2.000	0.29	77A
3-2	26 500.461(20)	26 500.4616(54)	3.000	0.88	77A
4-3	35 333.892(20)	35 333.8917(68)	4.000	1.77	77A
5-4		44 167.2728(78)	5.000	2.95	
6-5		53 000.5926(85)	6.000	4.42	
7-6		61 833.8390(88)	7.000	6.19	
8-7		70 666.9996(89)	8.000	8.25	
9-8		79 500.0620(88)	9.000	10.61	
10-9	88 535.002(35)	88 535.0141(89)	10.000	13.26	77A
11-10		97 165.8433(93)	11.000	16.21	
12-11		105 998.537(10)	12.000	19.45	
13-12	114 831.089(30)	114 831.084(11)	13.000	22.98	77A
14-13		123 663.471(12)	14.000	26.81	
15-14		132 495.685(13)	15.000	30.94	
16-15		141 327.714(14)	16.000	35.36	
17-16	150 159.546(40)	150 159.546(14)	17.000	40.07	77A
18-17		158 991.168(15)	18.000	45.08	
19-18		167 822.567(19)	19.000	50.38	
20-19	176 653.729(60)	176 653.731(28)	20.000	55.98	77A
21-20		185 484.646(43)	21.000	61.87	
22-21		194 315.302(64)	22.000	68.06	
23-22		203 145.683(92)	23.000	74.54	
24-23		211 975.78(13)	24.000	81.32	
25-24		220 805.57(17)	25.000	88.39	
26-25		229 635.06(23)	26.000	95.76	
27-26		238 464.22(30)	27.000	103.42	
28-27		247 293.04(38)	28.000	111.37	
29-28		256 121.51(48)	29.000	119.62	
30-29		264 949.61(60)	30.000	128.16	
31-30		273 777.33(73)	31.000	137.00	
32-31		282 604.67(89)	32.000	146.13	
33-32		291 431.6(11)	33.000	155.56	

Table 7., Rotational Spectrum of $D^{12}C^{12}C^{12}C^{14}N$ in the Ground State.

Transition J'-J''	F'-F''	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
1- 0			8 443.1615(9)	1.000	0.00	
	1- 1		8 442.0818 ^a	0.333		
	2- 1		8 443.3775	0.555		
	0- 1		8 445.3209	0.111		
2- 1			16 886.3122(17)	2.000	0.28	
	2- 2		16 885.0166	0.167		
	1- 0		16 885.2325	0.222		
	2- 1		16 886.3122	0.500		
	3- 2		16 886.4047	0.932		
	1- 2		16 887.1760	0.011		
	1- 1		16 888.4716	0.167		
3- 2		25 329.62(30)	25 329.4411(24)	3.000	0.84	50A
	3- 3		25 328.0529	0.111		
	2- 1		25 329.2252	0.600		
	3- 2		25 329.4411	0.888		
	4- 3		25 329.4925	1.287		
	2- 2		25 331.3846	0.111		
4- 3		33 772.532(50) ^b	33 772.5374(31)	4.000	1.69	
	4- 4	33 771.105(50) ^c	33 771.0978	0.083		77B
	3- 2		33 772.4449	0.952		
	4- 3	33 772.527(50) ^d	33 772.5374	1.252		77B
	5- 4		33 772.5701	1.628		
	3- 3	33 774.369(50) ^c	33 774.3883	0.083		77B
5- 4			42 215.5902(36)	5.000	2.82	
	5- 5		42 214.1179	0.067		
	4- 3		42 215.5388	1.295		
	5- 4		42 215.5902	1.600		
	6- 5		42 215.6129	1.970		
	4- 4		42 217.3897	0.067		
6- 5		50 658.598(12)	50 658.5887(40)	6.000	4.22	77B
	6- 6		50 657.0938	0.056		
	5- 4		50 658.5560	1.638		
	6- 5		50 658.5887	1.944		
	7- 6		50 658.6053	2.310		
	5- 5		50 660.3555	0.056		
7- 6		59 101.529(8)	59 101.5220(42)	7.000	5.91	77B
	7- 7		59 100.0104	0.048		
	6- 5		59 101.4994	1.974		
	7- 6		59 101.5220	2.289		
	8- 7		59 101.5347	2.646		
	6- 6		59 103.2661	0.048		

Table 7. Rotational Spectrum of $D^{12}C^{12}C^{12}C^{14}N$ in the Ground State (Continued).

Transition J'-J''	F'-F''	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
8-7		67 544.372(6)	67 544.3792(43)	8.000	7.89	77B
	8-8		67 542.8550	0.042		
	7-6		67 544.3626	2.312		
	8-7		67 544.3792	2.624		
	9-8		67 544.3893	2.984		
	7-7		67 546.1068	0.042		
9-8			75 987.1496(43)	9.000	10.14	
10-9			84 429.8221(43)	10.000	12.67	
11-10			92 872.3861(44)	11.000	15.49	
12-11			101 314.8307(47)	12.000	18.59	
13-12			109 757.1450(54)	13.000	21.97	
14-13			118 199.3183(63)	14.000	25.63	
15-14		126 641.343(8)	126 641.3397(74)	15.000	29.57	77B
16-15			135 083.1985(86)	16.000	33.80	
17-16			143 524.8839(98)	17.000	38.30	
18-17			151 966.385(11)	18.000	43.09	
19-18			160 407.691(12)	19.000	48.16	
20-19			168 848.792(12)	20.000	53.51	
21-20			177 289.676(12)	21.000	59.14	
22-21			185 730.333(11)	22.000	65.05	
23-22			194 170.7527(95)	23.000	71.25	
24-23		202 610.908(16)	202 610.9236(86)	24.000	77.73	77B
25-24		211 050.842(12)	211 050.835(10)	25.000	84.48	77B
26-25			219 490.477(16)	26.000	91.52	
27-26			227 929.839(25)	27.000	98.85	
28-27			236 368.910(37)	28.000	106.45	
29-28			244 807.679(52)	29.000	114.33	
30-29			253 246.136(71)	30.000	122.50	
31-30			261 684.270(95)	31.000	130.95	
32-31			270 122.07(12)	32.000	139.68	
33-32			278 559.53(16)	33.000	148.69	
34-33			286 996.63(19)	34.000	157.98	
35-34			295 433.37(24)	35.000	167.55	

^a Quadrupole hyperfine structure calculated assuming $eQq = -4.3188$ MHz. Uncertainties on the individual components should roughly follow the trend obtained for $H^{12}C^{12}C^{12}C^{14}N$ in Table 2.

^b Calculated from resolved components using $eQq = -4.3188$ MHz.

^c Lines used to calculate center frequency.

^d Not included in least-squares fitting.

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Table 8. Rotational Spectrum of $H^{12}C^{12}C^{12}C^{14}N$ in the ν_7^1 Vibrational State.

J'-J''	Transition F'-F''	$\ell'-\ell''$	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
2- 1		1e-1e		18 240.9520(67)	1.500	222.71	
	2- 1			18 239.8854(182)	0.375		
	2- 2			18 240.5254(100)	0.125		
	1- 1			18 240.9520(67)	0.125		
	3- 2			18 241.2110(72)	0.699		
	1- 2			18 241.5920(100)	0.008		
	1- 0			18 242.5519(236)	0.167		
2- 1		1f-1f		18 267.1045(67)	1.500	222.71	
	2- 1			18 266.0379(182)	0.375		
	2- 2			18 266.6779(100)	0.125		
	1- 1			18 267.1045(67)	0.125		
	3- 2			18 267.3635(72)	0.699		
	1- 2			18 267.7445(100)	0.008		
	1- 0			18 268.7044(236)	0.167		
3- 2		1e-1e		27 361.3944(100)	2.667	223.31	
	3- 3			27 360.4421(186)	0.099		
	3- 2		27 361.16(5)	27 361.1277(113)	0.789		77B
	2- 1 } 4- 3 }		27 361.54(5)*	27 361.5010(98) 27 361.5086(98)	0.533 1.144		77B
	2- 3			27 361.8819(186)	0.003		
	2- 2		27 362.59(5)	27 362.5676(186)	0.099		77B
3- 2		1f-1f		27 400.6222(100)	2.667	232.32	
	3- 3		27 399.69(5)	27 399.6699(186)	0.099		77B
	3- 2		27 400.35(5)	27 400.3555(113)	0.789		77B
	2- 1 } 4- 3 }		27 400.74(5)*	27 400.7288(98) 27 400.7364(98)	0.533 1.144		77B
	2- 3			27 401.1097(186)	0.003		
	2- 2			27 401.7954(186)	0.099		
4- 3		1e-1e		36 481.796(13)	3.750	224.23	
	4- 4			36 480.623(24)	0.078		
	4- 3			36 481.690(13)	1.174		
	3- 2		36 481.852(50)*	36 481.804(13)	0.893		77B
	5- 4			36 481.859(13)	1.526		
	3- 3		36 483.270(50)	36 483.244(23)	0.078		77B
4- 3		1f-1f		36 534.098(13)	3.750	224.23	
	4- 4		36 532.960(50)	36 532.925(24)	0.078		77B
	4- 3 } 3- 2 }		36 534.132(50)*	36 533.992(13) 36 534.106(13)	1.174 0.893		77B
	5- 4			36 534.161(13)	1.526		
	3- 3		36 535.548(50)	36 535.546(23)	0.078		77B

Table 8. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the ν_7^1 Vibrational State (Continued).

J'-J''	Transition		Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
	F'-F''	L'-L''					
5-4		1e-1e		45 602.145(16)	4.800	225.44	
	5-5			45 600.855(27)	0.064		
	5-4			45 602.091(16)	1.536		
	4-3			45 602.137(16)	1.243		
	6-5			45 602.184(16)	1.891		
	4-4			45 603.691(26)	0.064		
5-4		1f-1f		45 667.519(16)	4.800	225.45	
	5-5			45 666.229(27)	0.064		
	5-4			45 667.466(16)	1.536		
	4-3			45 667.511(16)	1.243		
	6-5			45 667.559(16)	1.891		
	4-4			45 669.066(26)	0.064		
6-5		1e-1e		54 722.425(19)	5.833	226.97	
	6-6			54 721.066(30)	0.054		
	6-5			54 722.395(19)	1.890		
	5-4			54 722.416(19)	1.593		
	7-6			54 722.452(19)	2.246		
	5-5			54 724.016(28)	0.054		
6-5		1f-1f		54 800.871(19)	5.833	226.97	
	6-6			54 799.511(30)	0.054		
	6-5			54 800.840(19)	1.890		
	5-4			54 800.861(19)	1.593		
	7-6			54 800.898(19)	2.246		
	5-5			54 802.461(28)	0.054		
7-6		1e-1e	63 842.60(10)	63 842.625(21)	6.857	228.79	77B
	7-7			63 841.220(32)	0.047		
	7-6			63 842.606(21)	2.242		
	6-5			63 842.616(21)	1.934		
	8-7			63 842.645(21)	2.592		
	6-6			63 844.237(29)	0.047		
7-6		1f-1f	63 934.18(10)	63 934.139(21)	6.857	228.80	77B
	7-7			63 932.733(32)	0.047		
	7-6			63 934.120(21)	2.242		
	6-5			63 934.130(21)	1.934		
	8-7			63 934.159(21)	2.592		
	6-6			63 935.751(29)	0.047		
8-7		1e-1e	72 962.70(10)	72 962.731(24)	7.875	230.92	77B
	8-8			72 961.294(34)	0.041		
	8-7			72 962.719(24)	2.583		
	7-6			72 962.723(24)	2.276		
	9-8			72 962.746(24)	2.937		
	7-7			72 964.354(31)	0.041		

Table 8. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the ν_7^1 Vibrational State (Continued).

J'-J''	Transition		Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
	F'-F''	K'-K''					
8-7	1f-1f		73 067.27(10)	73 067.311(24)	7.875	230.93	77B
	8-8			73 065.873(34)	0.041		
	8-7			73 067.298(24)	2.583		
	7-6			73 067.303(24)	2.276		
	9-8			73 067.325(24)	2.937		
	7-7			73 068.933(31)	0.041		
9-8	1e-1e			82 082.730(26)	8.889	233.35	
9-8	1f-1f			82 200.372(26)	8.889	233.37	
10-9	1e-1e		91 202.345(150)	91 202.607(27)	9.900	236.09	77C
10-9	1f-1f		91 333.415(110)	91 333.308(27)	9.900	236.11	77C
11-10	1e-1e			100 322.349(29)	10.909	239.13	
11-10	1f-1f			100 466.106(29)	10.909	239.16	
12-11	1e-1e			109 441.944(30)	11.917	242.48	
12-11	1f-1f			109 598.751(30)	11.917	242.51	
13-12	1e-1e			118 561.376(30)	12.923	246.13	
13-12	1f-1f			118 731.231(30)	12.923	246.17	
14-13	1e-1e		127 680.4(2)	127 680.634(31)	13.929	250.09	77B
14-13	1f-1f		127 863.4(2)	127 863.530(31)	13.929	250.13	77B
15-14	1e-1e			136 799.704(31)	14.933	254.35	
15-14	1f-1f			136 995.636(31)	14.933	254.39	
16-15	1e-1e			145 918.572(31)	15.938	258.91	
16-15	1f-1f			146 127.534(31)	15.938	258.96	
17-16	1e-1e			155 037.224(31)	16.941	263.78	
17-16	1f-1f			155 259.210(31)	16.941	263.83	
18-17	1e-1e			164 155.647(32)	17.944	268.95	
18-17	1f-1f			164 390.652(32)	17.944	269.01	
19-18	1e-1e			173 273.828(33)	18.947	274.42	
19-18	1f-1f			173 521.844(33)	18.947	274.50	
20-19	1e-1e			182 391.754(35)	19.950	280.20	
20-19	1f-1f			182 652.773(35)	19.950	280.29	
21-20	1e-1e			191 509.410(38)	20.952	286.29	
21-20	1f-1f			191 783.425(38)	20.952	286.38	
22-21	1e-1e			200 626.784(43)	21.955	292.67	
22-21	1f-1f	200 913.59(10)		200 913.786(43)	21.955	292.78	77B
23-22	1e-1e	209 744.02(10)		209 743.861(50)	22.957	299.37	77B
23-22	1f-1f	210 043.88(10)		210 043.843(50)	22.957	299.48	77B
24-23	1e-1e			218 860.629(58)	23.958	306.36	
24-23	1f-1f			219 173.582(58)	23.958	306.48	
25-24	1e-1e			227 977.074(68)	24.960	313.66	
25-24	1f-1f			228 302.988(68)	24.960	313.79	

Table 8. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the ν_7^1 Vibrational State (Continued).

J'-J''	Transition		Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
	F'-F''	$k'-k''$					
26-25		1e-1e		237 093.183(79)	25.962	321.27	
26-25		1f-1f		237 432.049(79)	25.962	321.41	
27-26		1e-1e		246 208.942(91)	26.963	329.18	
27-26		1f-1f		246 560.749(91)	26.963	329.33	
28-27		1e-1e		255 324.34(11)	27.964	337.39	
28-27		1f-1f		255 689.08(11)	27.964	337.55	
29-28		1e-1e		264 439.36(12)	28.966	345.91	
29-28		1f-1f		264 817.01(12)	28.966	346.08	
30-29		1e-1e		273 553.98(14)	29.967	354.73	
30-29		1f-1f		273 944.55(14)	29.967	354.92	
31-30		1e-1e		282 668.21(16)	30.968	363.85	
31-30		1f-1f		283 071.67(16)	30.968	364.05	
32-31		1e-1e		291 782.01(18)	31.969	373.28	
32-31		1f-1f		292 198.37(18)	31.969	373.50	
1- 1		1f-1e		13.0764(1)	1.500	222.71	
	0- 1			11.4766(238)	0.167		
	2- 1			12.4365(95)	0.209		
	1- 1	}		13.0764(1)	0.750		
	2- 2						
	2- 1			12.4365(95)	0.209		
	1- 0			14.6763(238)	0.167		
2- 2		1f-1e		39.2290(2)	0.833	223.32	
	2- 1			38.1624(159)	0.042		
	2- 3			38.5433(102)	0.043		
	1- 1	}		39.2290(2)	0.665		
	2- 2						
	3- 3						
	3- 2			39.9146(102)	0.043		
	1- 2			40.2955(159)	0.042		
3- 3		1f-1e		78.4568(4)	0.583	224.23	
	3- 2			77.0169(214)	0.015		
	3- 4			77.3902(159)	0.016		
	2- 2	}		78.4568(4)	0.522		
	3- 3						
	4- 4						
	4- 3			79.5233(159)	0.016		
	2- 3			79.8966(214)	0.015		
4- 4		1f-1e		130.7587(7)	0.450	225.44	
	4- 3			129.2045(231)	0.007		
	4- 5			129.5224(184)	0.007		
	3- 3	}		130.7587(7)	0.421		
	4- 4						
	5- 5						
	5- 4			131.9950(184)	0.007		
	3- 4			132.3129(231)	0.007		

Table 8. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the ν_7^1 Vibrational State (Continued).

J'-J''	Transition		Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency' (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
	F'-F''	k'-k''					
5-5		1f-1e		196.1332(10)	0.367	226.97	
	5-4			194.5334(238)	0.004		
	5-6			194.8041(198)	0.004		
	4-4	}		196.1332(10)	0.351		
	5-5						
	6-6						
	6-5			197.4624(198)	0.004		
	4-5			197.7331(238)	0.004		
6-6		1f-1e		274.5785(14)	0.310	228.79	
	6-5			272.9578(241)	0.002		
	6-7			273.1919(206)	0.002		
	5-5	}		274.5785(14)	0.305		
	6-6						
	7-7						
	7-6			275.9651(207)	0.002		
	5-6			276.1991(241)	0.002		
7-7		1f-1e		336.0921(18)	0.268	230.92	
8-8		1f-1e		470.6715(23)	0.236	233.35	
9-9		1f-1e		588.3134(29)	0.211	236.09	
10-10		1f-1e		719.0146(35)	0.191	239.13	
11-11		1f-1e		862.7711(41)	0.174	242.48	
12-12		1f-1e		1 019.5787(48)	0.160	246.13	
13-13		1f-1e		1 189.4329(56)	0.148	250.09	
14-14		1f-1e		1 372.3286(64)	0.138	254.35	
15-15		1f-1e		1 568.2604(72)	0.129	258.91	
16-16		1f-1e		1 777.2227(81)	0.121	263.78	
17-17		1f-1e		1 999.2093(89)	0.114	268.95	
18-18		1f-1e		2 234.2136(98)	0.108	274.42	
19-19		1f-1e		2 482.229(11)	0.103	280.20	
20-20		1f-1e		2 743.247(12)	0.098	286.29	
21-21		1f-1e		3 017.262(13)	0.093	292.67	
22-22		1f-1e		3 304.265(14)	0.089	299.37	
23-23		1f-1e		3 604.246(15)	0.085	306.36	
24-24		1f-1e		3 917.199(15)	0.082	313.66	
25-25		1f-1e		4 243.113(16)	0.078	321.27	
26-26		1f-1e		4 581.978(17)	0.075	329.18	
27-27		1f-1e		4 933.785(18)	0.073	337.39	
28-28		1f-1e		5 298.524(19)	0.070	345.91	
29-29		1f-1e		5 676.184(20)	0.068	354.73	
30-30		1f-1e		6 066.753(20)	0.066	363.85	
31-31		1f-1e		6 470.220(21)	0.064	373.28	
32-32		1f-1e		6 886.573(22)	0.062	383.01	
33-33		1f-1e		7 315.801(22)	0.060	393.05	
34-34		1f-1e		7 757.889(23)	0.058	403.39	
35-35		1f-1e	8 212.93(10)	8 212.826(23)	0.056	414.03	68A
36-36		1f-1e	8 680.72(10)	8 680.597(23)	0.055	424.98	68A
37-37		1f-1e	9 161.28(10)	9 161.190(23)	0.053	436.24	68A
38-38		1f-1e	9 654.62(10)	9 654.589(23)	0.052	447.79	68A

Table 8. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the ν_7^1 Vibrational State (Continued).

Transition J'-J''	F'-F'' K'-K''	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
39-39	1f-1e	10 160.80(10)	10 160.780(23)	0.051	459.65	68A
40-40	1f-1e	10 679.69(10)	10 679.749(23)	0.049	471.82	68A
41-41	1f-1e	11 211.50(10)	11 211.480(23)	0.048	484.28	68A
42-42	1f-1e	11 755.94(10)	11 755.956(22)	0.047	497.05	68A
43-43	1f-1e	12 313.21(10)	12 313.163(22)	0.046	510.13	68A
44-44	1f-1e	12 882.96(10)	12 883.084(22)	0.045	523.51	68A
45-45	1f-1e	13 465.70(10)	13 465.701(21)	0.044	537.20	68A
46-46	1f-1e		14 060.997(20)	0.043	551.18	
47-47	1f-1e	14 668.93(10)	14 668.955(20)	0.042	565.47	68A
48-48	1f-1e	15 289.43(10)	15 289.557(20)	0.041	580.07	68A
49-49	1f-1e	15 922.77(10)	15 922.785(20)	0.040	594.97	68A
50-50	1f-1e	16 568.53(10)	16 568.618(20)	0.040	610.17	68A
51-51	1f-1e	17 227.00(10)	17 227.040(21)	0.039	625.67	68A
52-52	1f-1e		17 898.029(23)	0.038	641.48	
53-53	1f-1e	18 581.56(10)	18 581.566(25)	0.037	657.59	68A
54-54	1f-1e	19 277.64(10)	19 277.630(27)	0.037	674.01	68A
55-55	1f-1e		19 986.201(31)	0.036	690.73	
56-56	1f-1e	20 707.31(10)	20 707.258(35)	0.035	707.75	68A
57-57	1f-1e	21 440.82(10)	21 440.779(39)	0.035	725.08	68A
58-58	1f-1e	22 186.79(10)	22 186.743(45)	0.034	742.71	68A
59-59	1f-1e		22 945.126(50)	0.034	760.65	
60-60	1f-1e		23 715.907(57)	0.033	778.88	

* Blended line not included in fitting.

Table 9. Rotational Spectrum of $H^{12}C^{12}C^{12}C^{14}N$ in the ν_6^1 Vibrational State.

Transition $J'-J''$ $F'-F''$ $k'-k''$	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
2- 1	1e-1e	18 226.036(12)	1.500	498.80	
2- 1		18 224.957 ^a	0.375		
2- 2		18 225.604	0.125		
1- 1		18 226.036	0.125		
3- 2		18 226.298	0.699		
1- 2		18 226.684	0.008		
1- 0		18 227.656	0.167		
2- 1	1f-1f	18 240.389(12)	1.500	498.80	
2- 1		18 239.310	0.375		
2- 2		18 239.957	0.125		
1- 1		18 240.389	0.125		
3- 2		18 240.652	0.699		
1- 2		18 241.037	0.008		
1- 0		18 242.009	0.167		
3- 2	1e-1e	27 339.22(20) ^b	2.667	499.41	
3- 3		27 338.059	0.099		
3- 2		27 338.93(10) ^c	0.789		77B
2- 1	}	27 339.22(10) ^d	0.533		77B
4- 3			1.144		
2- 3		27 339.517	0.003		
2- 2		27 340.211	0.099		
3- 2	1f-1f	27 360.59(20)	2.667	499.41	77B
3- 3		27 359.586	0.099		
3- 2		27 360.280	0.789		
2- 1		27 360.658	0.533		
4- 3		27 360.666	1.144		
2- 3		27 361.044	0.003		
2- 2		27 361.738	0.099		
4- 3	1e-1e	36 451.96(20)	3.750	500.32	77B
4- 4		36 450.785	0.078		
4- 3		36 451.865	1.174		
3- 2		36 451.980	0.893		
5- 4		36 452.037	1.526		
3- 3		36 453.438	0.078		
4- 3	1f-1f	36 480.62(20)	3.750	500.33	77B
4- 4		36 479.483	0.078		
4- 3		36 480.563	1.174		
3- 2		36 480.679	0.893		
5- 4		36 480.735	1.526		
3- 3		36 482.136	0.078		

Table 9. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the ν_6^1 Vibrational State (Continued).

Transition		Observed Frequency	Calculated Frequency	Line	Energy Level	Reference
J'-J''	F'-F''	(Est. Uncertainty)	(Est. Uncertainty)	Strength	of Lower State	
	L'-L''	in MHz	in MHz		(cm^{-1})	
5-4			45 564.872(24)	4.800	501.54	
	5-5		45 563.567	0.064		
	5-4		45 564.818	1.536		
	4-3		45 564.865	1.243		
	6-5		45 564.912	1.891		
	4-4		45 566.438	0.064		
5-4			45 600.738(25)	4.800	501.54	
	5-5		45 599.433	0.064		
	5-4		45 600.684	1.536		
	4-3		45 600.730	1.243		
	6-5		45 600.778	1.891		
	4-4		45 602.304	0.064		
6-5			54 677.710(27)	5.833	503.06	
	6-6		54 676.333	0.054		
	6-5		54 677.679	1.890		
	5-4		54 677.700	1.592		
	7-6		54 677.737	2.246		
	5-5		54 679.319	0.054		
6-5			54 720.738(28)	5.833	503.06	
	6-6		54 719.361	0.054		
	6-5		54 720.707	1.890		
	5-4		54 720.728	1.592		
	7-6		54 720.765	2.246		
	5-5		54 722.347	0.054		
7-6		63 790.44(10)	63 790.472(28)	6.857	504.88	77B
	7-7		63 789.049	0.054		
	7-6		63 790.453	1.890		
	6-5		63 790.463	1.592		
	8-7		63 790.492	2.246		
	6-6		63 792.103	0.047		
7-6		63 840.66(10)	63 840.657(29)	6.857	504.89	77B
	7-7		63 839.234	0.047		
	7-6		63 840.658	2.242		
	6-5		63 840.648	1.934		
	8-7		63 840.677	2.592		
	6-6		63 842.288	0.047		
8-7		72 903.20(10)	72 903.147(28)	7.875	507.01	77B
	8-8		72 901.692	0.041		
	8-7		72 903.134	2.583		
	7-6		72 903.139	2.276		
	9-8		72 903.162	2.937		
	7-7		72 904.790	0.041		

Table 9. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the ν_6^1 Vibrational State (Continued).

$J'-J''$	Transition $F'-F''$ $k'-k''$	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
8-7	1f-1f	72 960.48(10)	72 960.482(29)	7.875	507.02	
	8-8		72 959.026	0.041		
	8-7		72 960.469	2.583		
	7-6		72 960.474	2.276		
	9-8		72 960.497	2.937		
	7-7		72 962.124	0.041		
9-8	1e-1e		82 015.723(27)	8.889	509.44	
9-8	1f-1f		82 080.199(29)	8.889	509.45	
10-9	1e-1e	91 128.11(12)	91 128.186(28)	9.900	512.18	77C
10-9	1f-1f	91 199.80(15)	91 199.796(32)	9.900	512.19	77C
11-10	1e-1e		100 240.524(31)	10.909	515.22	
11-10	1f-1f		100 319.258(38)	10.909	515.23	
12-11	1e-1e		109 352.726(39)	11.917	518.56	
12-11	1f-1f		109 438.572(49)	11.917	518.58	
13-12	1e-1e	118 464.8(2)	118 464.777(53)	12.923	522.21	77C
13-12	1f-1f		118 557.724(66)	12.923	522.23	
14-13	1e-1e	127 576.7(2)	127 576.667(71)	13.929	526.16	77B
14-13	1f-1f	127 676.7(2)	127 676.703(88)	13.929	526.18	77B
15-14	1e-1e		136 688.382(95)	14.933	530.42	
15-14	1f-1f		136 795.492(115)	14.933	530.44	
16-15	1e-1e		145 799.91(12)	15.938	534.98	
16-15	1f-1f		145 914.08(15)	15.938	535.01	
17-16	1e-1e		154 911.24(16)	16.941	539.84	
17-16	1f-1f		155 032.45(19)	16.941	539.87	
18-17	1e-1e		164 022.35(20)	17.944	545.01	
18-17	1f-1f		164 150.60(23)	17.944	545.04	
19-18	1e-1e		173 133.25(24)	18.947	550.48	
19-18	1f-1f		173 268.50(28)	18.9407	550.52	
20-19	1e-1e		182 243.90(29)	19.950	556.25	
20-19	1f-1f		182 386.15(34)	19.95	556.30	
21-20	1e-1e		191 354.31(34)	20.952	562.33	
21-20	1f-1f		191 503.53(40)	20.952	562.38	
22-21	1e-1e		200 464.45(41)	21.955	568.72	
22-21	1f-1f		200 620.62(47)	21.955	568.77	

Table 9. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the ν_6^1 Vibrational State (Continued).

$J'-J''$	Transition $F'-F''$	$k'-k''$	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
23-22		1e-1e		209 574.32(47)	22.957	575.40	
23-22		1f-1f		209 737.42(55)	22.957	575.46	
24-23		1e-1e		218 683.90(55)	23.958	582.39	
24-23		1f-1f		218 853.91(63)	23.958	582.46	
25-24		1e-1e		227 793.19(63)	24.960	589.69	
25-24		1f-1f		227 970.08(73)	24.960	589.76	
26-25		1e-1e		236 902.16(72)	25.962	597.29	
26-25		1f-1f		237 085.91(83)	25.962	597.36	
27-26		1e-1e		246 010.80(82)	26.963	605.19	
27-26		1f-1f		246 201.40(94)	26.963	605.27	
28-27		1e-1e		255 119.11(92)	27.964	613.39	
28-27		1f-1f		255 316.52(105)	27.964	613.48	
29-28		1e-1e		264 227.1(10)	28.966	621.90	
29-28		1f-1f		264 431.3(12)	28.966	622.00	
30-29		1e-1e		273 334.7(12)	29.967	630.72	
30-29		1f-1f		273 545.6(13)	29.967	630.82	
31-30		1e-1e		282 441.9(13)	30.968	639.83	
31-30		1f-1f		282 659.6(15)	30.968	639.95	
32-31		1e-1e		291 548.7(14)	31.969	649.26	
32-31		1f-1f		291 773.1(16)	31.969	649.37	
1- 1		1f-1e		7.1770(85)	1.500	498.80	
	0- 1			5.5575	0.167		
	2- 1			6.5292	0.209		
	1- 1	}		7.1770	0.750		
	2- 2						
	1- 2			7.8248	0.209		
	1- 0			8.7966	0.167		
2- 2		1f-1e		21.530(25)	0.833	499.41	
	2- 1			20.450	0.042		
	2- 3			20.836	0.043		
	1- 1	}		21.530	0.663		
	2- 2						
	3- 3						
	3- 2			22.224	0.043		
	1- 2			22.610	0.042		

Table 9. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the ν_6^1 Vibrational State (Continued).

J'-J''	Transition F'-F'' & l'-l''	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
3-3	1f-1e		43.057(49)	0.583	500.32	
	3-2		41.600	0.015		
	3-4		41.978	0.016		
	2-2					
	3-3		43.057	0.522		
	4-4					
	4-3		44.137	0.016		
	2-3		44.515	0.015		
4-4	1f-1e		71.756(79)	0.450	501.54	
	4-3		70.182	0.007		
	4-5		70.504	0.007		
	3-3					
	4-4		71.756	0.421		
	5-5					
	5-4		73.007	0.007		
	3-4		73.329	0.007		
5-5	1f-1e		107.62(11)	0.367	503.06	
	5-4		106.00	0.004		
	5-6		106.28	0.004		
	4-4					
	5-5		107.62	0.351		
	6-6					
	6-5		108.97	0.004		
	4-5		109.24	0.004		
6-6	1f-1e		150.65(15)	0.310	504.88	
	6-5		149.01	0.002		
	6-7		149.25	0.002		
	5-5					
	6-6		150.65	0.300		
	7-7					
	7-6		152.05	0.002		
	5-6		152.29	0.002		
7-7	1f-1e		200.83(19)	0.268	507.01	
8-8	1f-1e		258.17(23)	0.236	509.44	
9-9	1f-1e		322.65(27)	0.211	512.18	
10-10	1f-1e		394.26(30)	0.191	515.22	
11-11	1f-1e		472.99(33)	0.174	518.56	
12-12	1f-1e		558.83(35)	0.160	522.21	
13-13	1f-1e		651.78(39)	0.148	526.16	
14-14	1f-1e		751.82(44)	0.138	530.42	
15-15	1f-1e		858.93(53)	0.129	534.98	

Table 9. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the ν_6^1 Vibrational State (Continued).

J'-J''	Transition		Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
	F'-F''	k'-k''					
16-16		1f-1e		973.10(66)	0.121	539.84	
17-17		1f-1e		1 094.31(86)	0.114	545.01	
18-18		1f-1e		1 222.6(11)	0.108	550.48	
19-19		1f-1e		1 357.8(15)	0.103	556.25	
20-20		1f-1e		1 500.1(19)	0.098	562.33	
21-21		1f-1e		1 649.3(24)	0.093	568.72	
22-22		1f-1e		1 805.5(30)	0.089	575.40	
23-23		1f-1e		1 968.6(37)	0.085	582.39	
24-24		1f-1e		2 138.6(45)	0.082	589.69	
25-25		1f-1e		2 315.5(55)	0.078	597.29	
26-26		1f-1e		2 499.2(66)	0.075	605.19	
27-27		1f-1e		2 689.8(78)	0.073	613.39	
28-28		1f-1e		2 887.2(92)	0.070	621.90	

^a Quadrupole hyperfine structure calculated assuming $eQq = -4.3188$ MHz. Uncertainties on the individual components should roughly follow the trend in Table 8.

^b Calculated from resolved hyperfine components using $eQq = -4.3188$ MHz.

^c Lines used to calculate center frequency.

^d Blended line not included in least-squares fitting.

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Table 10. Rotational Spectrum of $H^{12}C^{12}C^{12}C^{14}N$ in the v_5^1 Vibrational State.

Transition		Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
$J'-J''$	$l'-l''$					
2-1	1e-1e		18 197.932(22)	1.500	663.51	
	2-1		18 196.852 ^a	0.375		
	2-2		18 197.500	0.125		
	1-1		18 197.932	0.125		
	3-2		18 198.194	0.699		
	1-2		18 198.580	0.008		
	1-0		18 199.552	0.167		
2-1	1f-1f		18 208.254(22)	1.500	663.51	
	2-1		18 207.174	0.375		
	2-2		18 207.822	0.125		
	1-1		18 208.254	0.125		
	3-2		18 208.516	0.699		
	1-2		18 208.902	0.008		
	1-0		18 209.874	0.167		
3-2	1e-1e	27 297.14(20) ^h	27 296.857(32)	2.667	664.12	
	3-3		27 295.893	0.099		
	3-2	27 296.77(10) ^c	27 296.587	0.789		77B
	2-1 } 4-3 }	27 297.14(10) ^d	27 296.965	0.533		77B
	2-3		27 296.972	1.144		
	2-3		27 297.350	0.003		
	2-2		27 298.044	0.099		
3-2	1f-1f	27 312.55(20) ^b	27 312.335(32)	2.667	664.12	
	3-3		27 311.371	0.099		77B
	3-2	27 312.19(10) ^c	27 312.065	0.789		
	2-1 } 4-3 }	27 312.55(10) ^d	27 312.443	0.533		77B
	4-3		27 312.451	1.144		
	2-3		27 312.828	0.003		
	2-2		27 313.523	0.099		
4-3	1e-1e	36 395.80(10) ⁱ	36 395.732(40)	3.750	665.03	77B
	4-4		36 394.544	0.078		
	4-3		36 395.624	1.174		
	3-2		36 395.739	0.893		
	5-4		36 395.795	1.526		
	3-3		36 397.197	0.078		
4-3	1f-1f	36 416.39(10) ^j	36 416.360(41)	3.750	665.03	77B
	4-4		36 415.172	0.078		
	4-3		36 416.252	1.174		
	3-2		36 416.368	0.893		
	5-4		36 416.424	1.526		
	3-3		36 417.825	0.078		
5-4	1e-1e		45 494.540(47)	4.800	666.24	
	5-5		45 493.234	0.064		
	5-4		45 494.486	1.536		
	4-3		45 494.532	1.243		
	6-5		45 494.580	1.891		
	4-4		45 496.105	0.064		

Table 10. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the ν_5^1 Vibrational State (Continued).

Transition		Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
J'-J''	F'-F'' l'-l''					
5-4	1f-1f		45 520.311(48)	4.800	666.25	
	5-5		45 519.006	0.064		
	5-4		45 520.257	1.536		
	4-3		45 520.303	1.243		
	6-5		45 520.351	1.891		
	4-4		45 521.877	0.064		
6-5	1e-1e		54 593.265(51)	5.833	667.76	
	6-6		54 591.889	0.054		
	6-5		54 593.235	1.890		
	5-4		54 593.256	1.593		
	7-6		54 593.293	2.246		
	5-5		54 594.875	0.054		
6-5	1f-1f		54 624.170(53)	5.833	667.76	
	6-6		54 622.793	0.054		
	6-5		54 624.139	1.890		
	5-4		54 624.160	1.593		
	7-6		54 624.197	2.246		
	5-5		54 625.779	0.054		
7-6	1e-1e	63 691.91(10)	63 691.891(54)	6.857	669.58	77B
	7-7		63 690.468	0.047		
	7-6		63 691.872	2.242		
	6-5		63 691.882	1.934		
	8-7		63 691.911	2.592		
	6-6		63 693.523	0.047		
7-6	1f-1f	63 727.97(10)	63 727.917(56)	6.857	669.59	77B
	7-7		63 726.494	0.047		
	7-6		63 727.898	2.242		
	6-5		63 727.908	1.934		
	8-7		63 727.937	2.592		
	6-6		63 729.548	0.047		
8-7	1e-1e	72 790.30(10)	72 790.401(55)	7.875	671.71	77B
	8-8		72 788.945	0.041		
	8-7		72 790.388	2.583		
	7-6		72 790.393	2.276		
	9-8		72 790.416	2.937		
	7-7		72 792.044	0.041		
8-7	1f-1f	72 831.42(10)	72 831.535(58)	7.875	671.71	77B
	8-8		72 830.079	0.041		
	8-7		72 831.522	2.583		
	7-6		72 831.527	2.276		
	9-8		72 831.550	2.937		
	7-7		72 833.177	0.041		

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Table 10. Rotational Spectrum of $H^{12}C^{12}C^{12}C^{14}N$ in the ν_5^1 Vibrational State (Continued).

$J'-J''$	Transition $F'-F''$ $\lambda'-\lambda''$	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
9-8	1e-1e		81 888.778(56)	8.889	674.14	
9-8	1f-1f		81 935.004(59)	8.889	674.14	
10-9	1e-1e	90 986.97(20)	90 987.005(58)	9.900	676.87	77C
10-9	1f-1f		91 038.307(61)	9.900	676.87	
11-10	1e-1e		100 085.067(66)	10.909	679.90	
11-10	1f-1f		100 141.425(69)	10.909	679.91	
12-11	1e-1e		109 182.946(81)	11.917	683.24	
12-11	1f-1f		109 244.339(84)	11.917	683.25	
13-12	1e-1e	118 280.70(20)	118 280.63(11)	12.923	686.88	77C
13-12	1f-1f	118 347.20(20)	118 347.03(11)	12.923	686.90	77C
14-13	1e-1e	127 378.10(20)	127 378.09(14)	13.929	690.83	77B
14-13	1f-1f	127 449.40(20)	127 449.48(14)	13.929	690.84	77B
15-14	1e-1e		136 475.32(19)	14.933	695.08	
15-14	1f-1f		136 551.67(19)	14.933	695.09	
16-15	1e-1e		145 572.30(24)	15.938	699.63	
16-15	1f-1f		145 653.59(24)	15.938	699.65	
17-16	1e-1e		154 669.02(30)	16.941	704.48	
17-16	1f-1f		154 755.20(30)	16.941	704.51	
18-17	1e-1e		163 765.46(37)	17.944	709.64	
18-17	1f-1f		163 856.51(38)	17.944	709.67	
19-18	1e-1e		172 861.59(46)	18.947	715.11	
19-18	1f-1f		172 957.48(46)	18.947	715.14	
20-19	1e-1e		181 957.41(55)	19.950	720.87	
20-19	1f-1f		182 058.09(55)	19.950	720.90	
21-20	1e-1e		191 052.90(66)	20.952	726.94	
21-20	1f-1f		191 158.34(66)	20.952	726.98	
22-21	1e-1e		200 148.04(77)	21.955	733.31	
22-21	1f-1f		200 258.20(77)	21.955	733.53	
23-22	1e-1e		209 242.82(90)	22.957	739.99	
23-22	1f-1f		209 357.65(90)	22.957	740.03	
24-23	1e-1e		218 337.2(10)	23.958	746.97	
24-23	1f-1f		218 456.7(10)	23.958	747.02	
25-24	1e-1e		227 431.2(12)	24.960	754.25	
25-24	1f-1f		227 555.3(12)	24.960	754.30	
26-25	1e-1e		236 524.8(14)	25.962	761.84	
26-25	1f-1f		236 653.4(14)	25.962	761.89	
27-26	1e-1e		245 617.9(15)	26.963	769.73	
27-26	1f-1f		245 751.0(15)	26.963	769.79	
28-27	1e-1e		254 710.0(17)	27.964	777.92	
28-27	1f-1f		254 848.1(17)	27.964	777.99	

Table 10. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the ν_5^1 Vibrational State (Continued).

Transition		Observed Frequency	Calculated Frequency	Line	Energy Level	Reference
$J'-J''$	$F'-F''$	(Est. Uncertainty)	(Est. Uncertainty)	Strength	of Lower State	
	$k'-k''$	in MHz	in MHz		(cm^{-1})	
29-28		1e-1e	263 802.9(20)	28.966	786.42	
29-28		1f-1f	263 944.8(20)	28.966	786.49	
30-29		1e-1e	272 894.6(22)	29.967	795.22	
30-29		1f-1f	273 040.8(22)	29.967	795.29	
31-30		1e-1e	281 985.9(24)	30.968	804.32	
31-30		1f-1f	282 136.4(24)	30.968	804.40	
32-31		1e-1e	291 076.6(27)	31.969	813.73	
32-31		1f-1f	291 231.3(27)	31.969	813.81	
1- 1		1f-1e	5.162(16)	1.500	663.51	
	0- 1		3.542	0.167		
	2- 1		4.514	0.209		
	1- 1		5.162	0.750		
	2- 2					
	1- 2		5.810	0.209		
	1- 0		6.782	0.167		
2- 2		1f-1e	15.484(47)	0.833	664.12	
	2- 1		14.404	0.042		
	2- 3		14.790	0.043		
	1- 1					
	2- 2		15.484	0.633		
	3- 3					
	3- 2		16.178	0.043		
	1- 2		16.564	0.042		
3-3		1f-1e	30.962(92)	0.583	665.03	
	3- 2		29.505	0.015		
	3- 4		29.882	0.016		
	2- 2					
	3- 3		30.962	0.522		
	4- 4					
	4- 3		32.042	0.016		
	2- 3		32.426	0.015		
4- 4		1f-1e	51.59(15)	0.450	666.24	
	4- 3		50.02	0.007		
	4- 5		50.34	0.007		
	3- 3					
	4- 4		51.59	0.421		
	5- 5					
	5- 4		52.84	0.007		
	3- 4		53.16	0.007		
5- 5		1f-1e	77.36(22)	0.367	667.76	
	5- 4		75.74	0.004		
	5- 6		76.02	0.004		
	4- 4					
	5- 5		77.36	0.351		
	6- 6					
	6- 5		78.71	0.004		
	4- 5		78.98	0.004		

Table 10. Rotational Spectrum of $H^{12}C^{12}C^{12}C^{14}N$ in the ν_5^1 Vibrational State (Continued).

J'-J''	Transition		Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
	F'-F''	ℓ' - ℓ''					
6-6		1f-1e		108.27(29)	0.310	669.58	
	6-5			106.63	0.002		
	6-7			106.86	0.002		
	5-5						
	6-6			108.27	0.305		
	7-7						
	7-6			109.67	0.002		
	5-6			109.91	0.002		
7-7		1f-1e		144.29(37)	0.261	671.71	
8-8		1f-1e		185.43(44)	0.281	674.14	
9-9		1f-1e		231.65(52)	0.211	676.87	
10-10		1f-1e		282.95(58)	0.191	679.91	
11-11		1f-1e		339.31(65)	0.174	683.24	
12-12		1f-1e		400.71(71)	0.160	686.90	
13-13		1f-1e		467.11(78)	0.148	690.83	
14-14		1f-1e		538.50(88)	0.138	695.08	
15-15		1f-1e		614.9(10)	0.129	699.63	
16-16		1f-1e		696.1(13)	0.121	704.48	
17-17		1f-1e		782.3(16)	0.114	709.64	
18-18		1f-1e		873.4(20)	0.108	715.10	
19-19		1f-1e		969.3(26)	0.103	720.87	
20-20		1f-1e		1 069.9(33)	0.098	726.94	
21-21		1f-1e		1 175.4(42)	0.093	733.31	
22-22		1f-1e		1 285.5(52)	0.089	739.99	
23-23		1f-1e		1 400.4(65)	0.085	746.97	
24-24		1f-1e		1 519.8(80)	0.082	754.25	
25-25		1f-1e		1 643.9(96)	0.078	761.84	

^a Quadrupole hyperfine structure calculated assuming $eQq = -4.3188$ MHz. Uncertainties on the individual components should roughly follow the trend in Table 8.

^b Calculated from resolved components using $eQq = -4.3188$ MHz.

^c Lines used to calculate center frequency.

^d Blended line not included in least-squares fitting.

Table 11. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the $2\nu_7^0$ and $2\nu_7^2$ Vibrational States.

Transition J'-J''	F'-F''	K'-K''	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
1-0		0-0	9 155.92(10) ^b	9 155.9391(55) ^a	1.000	443.36	
	1-1		9 154.88(10) ^c	9 154.8595	0.333		63A
	2-1		9 156.09(10) ^c	9 156.1551	0.555		63A
	0-1			9 158.0985	0.111		
2-1		0-0		18 311.849(11)	2.000	443.67	
	2-2			18 310.553	0.167		
	1-0			18 310.769	0.222		
	2-1			18 311.849	0.500		
	3-2			18 311.941	0.932		
	1-2			18 312.713	0.011		
	1-1			18 314.008	0.167		
3-2		0-0		27 467.699(16)	3.000	444.28	
	3-3			27 466.311	0.111		
	2-1			27 467.483	0.600		
	3-2		27 467.68(15) ^d	27 467.699	0.888		77B
	4-3			27 467.751	1.287		
	2-2			27 469.643	0.111		
3-2		2e-2e		27 467.433(17)	1.667	446.10	
	3-2			27 466.353	0.555		
	2-2						
	4-3						
	3-3		27 467.68(15) ^d	27 467.742	0.778		77B
	2-3						
	2-1			27 468.513	0.383		
3-2		2F-2F		27 467.494(17)	1.667	446.10	
	3-2			27 466.414	0.555		
	2-2						
	4-3						
	3-3		27 467.68(15) ^d	27 467.802	0.778		77B
	2-3						
	2-1			27 468.573	0.333		
4-3		0-0		36 623.461(21)	4.000	445.20	
	4-4			36 622.022	0.083		
	3-2			36 623.369	0.952		
	4-3		36 623.34(10) ^d	36 623.461	1.252		77B
	5-4			36 623.494	1.628		
	3-3			36 625.312	0.083		
4-3		2e-2e		36 623.177(23)	3.000	447.01	
	4-3		36 622.88(10) ^d	36 622.745	1.001		77B
	4-4						
	5-4		36 623.34(10) ^d	36 623.334	1.221		77B
	3-2						
	3-3			36 623.486	0.777		
	3-4						

Table 11. Rotational Spectrum of $H^{12}C^{12}C^{12}C^{14}N$ in the $2\nu_7^0$ and $2\nu_7^2$ Vibrational States (Continued).

$J'-J''$	Transition $F'-F''$ $l'-l''$	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
4-3	2f-2f		36 623.329(23)	3.000	447.01	
	4-3 } 4-4 }	36 622.88(10) ^d	36 622.897	1.001		77B
	5-4	36 623.34(10) ^d	36 623.486	1.221		77B
	3-2 } 3-3 }		36 623.637	0.777		
	3-4 }					
5-4	0-0		45 779.105(26)	5.000	446.42	
	5-5		45 777.633	0.067		
	4-3		45 779.054	1.295		
	5-4		45 779.105	1.600		
	6-5		45 779.128	1.970		
	4-4		45 780.905	0.067		
5-4	2e-2e		45 778.864(28)	4.200	448.23	
	5-5		45 778.059	0.056		
	5-4		45 778.648	1.344		
	6-5		45 778.956	1.655		
	4-3		45 778.987	1.088		
	4-4		45 779.727	0.056		
5-4	2f-2f		45 779.167(28)	4.200	448.23	
	5-5		45 778.362	0.056		
	5-4		45 778.951	1.344		
	6-5		45 779.259	1.655		
	4-3		45 779.290	1.088		
	4-4		45 780.030	0.056		
6-5	0-0		54 934.602(30)	6.000	447.95	
	6-6		54 933.107	0.056		
	5-4		54 934.569	1.638		
	6-5		54 934.602	1.944		
	7-6		54 934.618	2.310		
	5-5		54 936.369	0.056		
6-5	2e-2e		54 934.478(33)	5.333	449.76	
	6-6		54 933.458	0.049		
	6-5		54 934.355	1.728		
	5-4		54 934.537	1.456		
	7-6		54 934.538	2.053		
	5-5		54 935.617	0.049		
6-5	2f-2f		54 935.009(32)	5.333	449.76	
	6-6		54 933.988	0.049		
	6-5		54 934.885	1.728		
	5-4		54 935.068	1.456		
	7-6		54 935.068	2.053		
	5-5		54 936.147	0.049		

Table 11. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the $2\nu_7^0$ and $2\nu_7^2$ Vibrational States (Continued).

J'-J''	Transition		Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
	F'-F''	$\ell'-\ell''$					
7-6		0-0	64 089.87(10) ^d	64 089.921(34)	7.000	449.78	77B
		7-7		64 088.410	0.048		
		6-5		64 089.899	1.974		
		7-6		64 089.921	2.289		
		8-7		64 089.934	2.646		
		6-6		64 091.665	0.048		
7-6		2e-2e	64 089.87(10) ^d	64 090.007(38)	6.429	451.59	
		7-7		64 088.850	0.044		
		7-6		64 089.930	2.102		
		6-5		64 090.038	1.813		
		8-7		64 090.048	2.430		
		6-6		64 091.300	0.044		
7-6		2f-2f	64 090.77(10)	64 090.855(36)	6.429	451.59	
		7-7		64 089.699	0.044		
		7-6		64 090.778	2.102		
		6-5		64 090.887	1.813		
		8-7		64 090.896	2.430		
		6-6		64 092.149	0.044		
8-7		0-0	73 245.21(10) ^d	73 245.034(38)	8.000	451.92	
		8-8		73 243.510	0.042		
		7-6		73 245.017	2.312		
		8-7		73 245.034	2.624		
		9-8		73 245.044	2.984		
		7-7		73 246.761	0.042		
8-7		2e-2e	73 245.21(10) ^d	73 245.435(42)	7.500	453.73	
		8-8		73 244.186	0.039		
		8-7		73 245.383	2.460		
		7-6		73 245.453	2.168		
		9-8		73 245.464	2.798		
		7-7		73 246.823	0.039		
8-7		2f-2f	73 246.63(10)	73 246.708(40)	7.500	453.73	
		8-8		73 245.459	0.039		
		8-7		73 246.656	2.460		
		7-6		73 246.726	2.168		
		9-8		73 246.737	2.798		
		7-7		73 248.096	0.039		
9-8		0-0		82 399.910(41)	9.000	454.36	
9-8		2e-2e		82 400.748(46)	8.556	456.17	
9-8		2f-2f		82 402.566(43)	8.556	456.17	
10-9		0-0		91 554.521(43)	10.000	457.11	
10-9		2e-2e	91 556.03(11)	91 555.932(49)	9.600	458.92	77C
10-9		2f-2f	91 558.19(11)	91 558.432(45)	9.600	458.92	77C

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Table 11. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the $2\nu_2^0$ and $2\nu_2^2$ Vibrational States (Continued).

$J'-J''$	Transition		Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
	$F'-F''$	$k'-k''$					
11-10		0-0		100 708.837(45)	11.000	460.16	
11-10		2e-2e		100 710.972(52)	10.636	461.98	
11-10		2f-2f		100 714.306(47)	10.636	461.98	
12-11		0-0		109 862.828(46)	12.000	463.52	
12-11		2e-2e		109 865.854(55)	11.667	465.34	
12-11		2f-2f		109 870.188(48)	11.667	465.34	
13-12		0-0	119 016.50(5)	119 016.465(47)	13.000	467.18	77C
13-12		2e-2e	119 020.80(20)	119 020.564(56)	12.692	469.00	77C
13-12		2f-2f	119 026.24(20)	119 026.080(49)	12.692	469.00	77C
14-13		0-0	128 169.7(2)	128 169.718(48)	14.000	471.15	77B
14-13		2e-2e	128 175.1(2)	128 175.088(58)	13.714	472.97	77B
14-13		2f-2f	128 182.0(2)	128 181.982(49)	13.714	472.97	77B
15-14		0-0		137 322.558(48)	15.000	475.43	
15-14		2e-2e		137 329.410(59)	14.733	477.25	
15-14		2f-2f		137 337.896(50)	14.733	477.25	
16-15		0-0		146 474.956(49)	16.000	480.01	
16-15		2e-2e		146 483.516(60)	15.750	481.83	
16-15		2f-2f		146 493.821(51)	15.750	481.83	
17-16		0-0		155 626.881(51)	17.000	484.90	
17-16		2e-2e		155 637.393(61)	16.765	486.71	
17-16		2f-2f		155 649.759(53)	16.765	486.72	
18-17		0-0		164 778.304(55)	18.000	490.09	
18-17		2e-2e		164 791.026(63)	17.778	491.91	
18-17		2f-2f		164 805.710(57)	17.778	491.91	
19-18		0-0		173 929.196(60)	19.000	495.58	
19-18		2e-2e		173 944.400(65)	18.789	497.40	
19-18		2f-2f		173 961.676(63)	18.789	497.40	
20-19		0-0		183 079.527(68)	20.000	501.39	
20-19		2e-2e		183 097.502(65)	19.800	503.20	
20-19		2f-2f		183 117.656(73)	19.800	503.21	
21-20		0-0		192 229.268(79)	21.000	507.49	
21-20		2e-2e		192 250.316(73)	20.810	509.31	
21-20		2f-2f		192 273.652(85)	20.810	509.32	
22-21		0-0	201 378.31(10)	201 378.389(93)	22.000	513.90	77B
22-21		2e-2e	201 402.91(10)	201 402.828(80)	21.818	515.72	77B
22-21		2f-2f	201 429.63(10)	201 429.665(101)	21.818	515.73	77B
23-22		0-0		210 526.860(109)	23.000	520.62	
23-22		2e-2e		210 555.025(89)	22.826	522.44	
23-22		2f-2f		210 585.696(119)	22.826	522.45	

Table 11. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the $2\nu_7^0$ and $2\nu_7^2$ Vibrational States (Continued).

J'-J''	Transition		Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
	F'-F''	K'-K''					
24-23		0-0		219 674.65(13)	24.000	527.64	
24-23		2e-2e		219 706.89(10)	23.833	529.47	
24-23		2f-2f		219 741.74(14)	23.833	529.47	
25-24		0-0		228 821.74(15)	25.000	534.97	
25-24		2e-2e		228 858.41(11)	24.840	536.79	
25-24		2f-2f		228 897.81(16)	24.840	536.80	
26-25		0-0		237 968.08(17)	26.000	542.60	
26-25		2e-2e		238 009.57(13)	25.846	544.43	
26-25		2f-2f		238 053.90(19)	25.846	544.44	
27-26		0-0		247 113.66(20)	27.000	550.54	
27-26		2e-2e		247 160.36(15)	26.852	552.37	
27-26		2f-2f		247 210.01(22)	26.852	552.38	
28-27		0-0		256 258.45(23)	28.000	558.79	
28-27		2e-2e		256 310.77(17)	27.857	560.61	
28-27		2f-2f		256 366.14(25)	27.857	560.62	
29-28		0-0		265 402.40(26)	29.000	567.33	
29-28		2e-2e		265 460.76(19)	28.862	569.16	
29-28		2f-2f		265 522.29(29)	28.862	569.18	
30-29		0-0		274 545.50(30)	30.000	576.19	
30-29		2e-2e		274 610.35(22)	29.867	578.02	
30-29		2f-2f		274 678.46(33)	29.867	578.03	
31-30		0-0		283 687.71(34)	31.000	585.34	
31-30		2e-2e		283 759.50(25)	30.871	587.18	
31-30		2f-2f		283 834.66(37)	30.871	587.19	
32-31		0-0		292 829.01(38)	32.000	594.81	
32-31		2e-2e		292 908.21(28)	31.875	596.64	
32-31		2f-2f		292 990.88(42)	31.875	596.66	
33-32		0-0		301 969.37(42)	33.000	604.57	
33-32		2e-2e		302 056.45(31)	32.879	606.41	
33-32		2f-2f		302 147.13(47)	32.879	606.44	

^a Quadrupole hyperfine structure calculated assuming $eQq = -4.3188$ MHz.

^b Calculated from resolved hyperfine components using $eQq = -4.3188$ MHz.

^c Lines used to calculate center frequency.

^d Blended line not included in least-squares fitting.

MICROWAVE SPECTRUM OF CYANOACETYLENE

Table 12. Rotational Spectrum of $H^{12}C^{12}C^{12}C^{14}N$ in the $3v_7^1$ Vibrational State.

Transition J'-J''	F'-F''	$\lambda'-\lambda''$	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
2- 1		1e-1e		18 342.438(17)	1.500	665.01	
	2- 1			18 341.359 ^a	0.375		
	2- 2			18 342.007	0.125		
	1- 1			18 342.438	0.125		
	3- 2			18 342.701	0.699		
	1- 2			18 343.086	0.008		
	1- 0			18 344.058	0.167		
2- 1		1f-1f		18 395.090(17)	1.500	665.01	
	2- 1			18 394.010	0.375		
	2- 2			18 394.658	0.125		
	1- 1			18 395.090	0.125		
	3- 2			18 395.352	0.699		
	1- 2			18 395.738	0.008		
	1- 0			18 396.709	0.167		
3- 2		1e-1e	27 513.729(50) ^b	27 513.623(24)	2.667	665.62	
	3- 3		27 512.790(50) ^c	27 512.659	0.099		77B
	3- 2		27 513.470(50) ^c	27 513.353	0.789		77B
	2- 1	}	27 513.840(50) ^d	27 513.731	0.533		77B
	4- 3			27 513.739	1.144		
	2- 3			27 514.117	0.003		
	2- 2		27 514.880(50) ^c	27 514.811	0.009		77B
3- 2		1f-1f	27 592.483(50) ^b	27 592.599(24)	2.667	665.62	
	3- 3		27 591.580(50) ^c	27 591.635	0.099		77B
	3- 2		27 592.240(50) ^c	27 592.329	0.789		77B
	2- 1	}	27 592.600(100) ^d	27 592.707	0.533		77B
	4- 3			27 592.715	1.144		
	2- 3			27 593.092	0.003		
	2- 2		27 593.630(50) ^c	27 593.787	0.099		77B
4- 3		1e-1e	36 684.882(50) ^b	36 684.766(31)	3.750	666.54	
	4- 4		36 683.714(50) ^c	36 683.578	0.078		77B
	4- 3	}	36 684.905(100)	36 684.658	1.174		77B
	3- 2			36 684.774	0.893		
	5- 4			36 684.830	1.526		
	3- 3		36 686.327(50)	36 686.231	0.078		77B
4- 3		1f 1f	36 789.957(50)	36 790.064(31)	3.750	666.54	
	4- 4		36 788.810(50)	36 788.877	0.078		77B
	4- 3	}	36 789.976(100)	36 789.957	1.174		77B
	3- 2			36 790.072	0.893		
	5- 4			36 790.128	1.526		
	3- 3		36 791.381(50)	36 791.530	0.078		77B
5- 4		1e-1e		45 855.853(36)	4.800	667.76	
	5- 5			45 854.548	0.064		
	5- 4			45 855.799	1.536		
	4- 3			45 855.846	1.243		
	6- 5			45 855.893	1.891		
	4- 4			45 857.419	0.064		

Table 12. Rotation Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the $3\nu_7^1$ Vibrational State (Continued).

J'-J''	F'-F''	$\lambda'-\lambda''$	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
5-4		1f-1f		45 987.472(36)	4.800	667.77	
	5-5			45 986.167	0.064		
	5-4			45 987.418	1.536		
	4-3			45 987.465	1.243		
	6-5			45 987.512	1.891		
	4-4			45 989.038	0.064		
6-5		1e-1e		55 026.872(39)	5.833	669.29	
	6-6			55 025.495	0.054		
	6-5			55 026.841	1.890		
	5-4			55 026.862	1.592		
	7-6			55 026.899	2.246		
	5-5			55 028.482	0.054		
6-5		1f-1f		55 184.808(39)	5.833	669.30	
	6-6			55 183.432	0.054		
	6-5			55 184.777	1.890		
	5-4			55 184.798	1.592		
	7-6			55 184.835	2.246		
	5-5			55 186.418	0.054		
7-6		1e-1e	64 197.89(10)	64 197.807(41)	6.857	671.13	77B
	7-7			64 196.384	0.047		
	7-6			64 197.788	2.242		
	6-5			64 197.798	1.934		
	8-7			64 197.827	2.592		
	6-6			64 199.439	0.047		
7-6		1f-1f	64 389.96(10)	64 382.057(41)	6.857	671.14	77B
	7-7			64 380.634	0.047		
	7-6			64 382.037	2.242		
	6-5			64 382.047	1.934		
	8-7			64 382.076	2.592		
	6-6			64 383.688	0.047		
8-7		1e-1e	73 368.76(10)	73 368.646(44)	7.875	673.27	77B
	8-8			73 367.191	0.041		
	8-7			73 368.633	2.583		
	7-6			73 368.638	2.276		
	9-8			73 368.661	2.937		
	7-7			73 370.289	0.041		
8-7		1f-1f	73 579.07(10)	73 579.204(44)	7.875	673.29	77B
	8-8			73 577.748	0.041		
	8-7			73 579.191	2.583		
	7-6			73 579.196	2.276		
	9-8			73 579.219	2.937		
	7-7			73 580.847	0.041		

Table 12. Rotation Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the $3\nu_7^1$ Vibrational State (Continued).

J'-J''	Transition		Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
	F'-F''	$k'-k''$					
9- 8		1e-1e		82 539.375(47)	8.889	675.71	
	9- 9			82 537.895	0.037		
	9- 8			82 539.366	2.924		
	8- 7			82 539.368	2.613		
	10- 9			82 539.386	3.271		
	8- 8			82 541.023	0.037		
9- 8		1f-1f		82 776.235(47)	8.889	675.75	
	9- 9			82 774.756	0.037		
	9- 8			82 776.226	2.924		
	8- 7			82 776.228	2.613		
	10- 9			82 776.247	3.271		
	8- 8			82 777.884	0.037		
10- 9		1e-1e	91 710.02(15)	91 709.980(55)	9.900	678.47	77C
10- 9		1f-1f	91 973.18(15)	91 973.135(55)	9.900	678.51	77C
11-10		1e-1e		100 880.448(70)	10.909	681.53	
11-10		1f-1f		101 169.890(70)	10.909	681.58	
12-11		1e-1e		110 050.765(92)	11.917	684.89	
12-11		1f-1f		110 366.484(92)	11.917	684.95	
13-12		1e-1e	119 220.84(30)	119 220.92(12)	12.923	688.56	77C
13-12		1f-1f	119 562.90(10)	119 562.90(12)	12.923	688.63	77C
14-13		1e-1e		128 390.90(16)	13.929	692.54	
14-13		1f-1f		128 759.13(16)	13.929	692.62	
15-14		1e-1e		137 560.68(21)	14.933	696.82	
15-14		1f-1f		137 955.15(21)	14.933	696.92	
16-15		1e-1e		146 730.27(26)	15.938	701.41	
16-15		1f-1f		147 150.95(26)	15.938	701.52	
17-16		1e-1e		155 899.64(32)	16.941	706.31	
17-16		1f-1f		156 346.52(32)	16.941	706.43	
18-17		1e-1e		165 068.78(40)	17.944	711.51	
18-17		1f-1f		165 541.83(40)	17.944	711.64	
19-18		1e-1e		174 237.68(48)	18.947	717.01	
19-18		1f-1f		174 736.87(48)	18.947	717.16	
20-19		1e-1e		183 406.33(57)	19.950	722.82	
20-19		1f-1f		183 931.63(57)	19.950	722.99	
21-20		1e-1e		192 574.72(67)	20.952	728.94	
21-20		1f-1f		193 126.09(67)	20.952	729.13	
22-21		1e-1e		201 742.82(79)	21.955	735.37	
22-21		1f-1f		202 320.23(79)	21.955	735.57	

Table 12. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the $3\nu_7^1$ Vibrational State (Continued).

J'-J''	Transition		Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
	F'-F''	L'-L''					
23-22		1e-1e		210 910.65(91)	22.957	742.09	
23-22		1f-1f		211 514.04(91)	22.957	742.32	
24-23		1e-1e		220 078.2(10)	23.952	749.13	
24-23		1f-1f		220 707.5(10)	23.958	749.37	
25-24		1e-1e		229 245.4(12)	24.960	756.47	
25-24		1f-1f		229 900.6(12)	24.960	756.73	
26-25		1e-1e		238 412.3(14)	25.962	764.12	
26-25		1f-1f		239 093.3(14)	25.962	764.40	
27-26		1e-1e		247 578.8(15)	26.963	772.07	
27-26		1f-1f		248 285.6(15)	26.963	772.38	
28-27		1e-1e		256 745.0(17)	27.964	780.33	
28-27		1f-1f		257 477.5(17)	27.964	780.66	
29-28		1e-1e		265 910.9(19)	28.966	788.89	
29-28		1f-1f		266 668.9(19)	28.966	789.25	
30-29		1e-1e		275 076.4(22)	29.967	797.76	
30-29		1f-1f		275 859.9(22)	29.967	798.14	
31-30		1e-1e		284 241.5(24)	30.968	806.94	
31-30		1f-1f		285 050.5(24)	30.968	807.35	
32-31		1e-1e		293 406.3(26)	31.969	816.42	
32-31		1f-1f		294 240.5(26)	31.969	816.85	
1-1		1f-1e		26.326(1)	1.500	665.01	
2-2		1f-1e		78.978(2)	0.833	665.62	
3-3		1f-1e		157.953(4)	0.583	666.54	
4-4		1f-1e		263.252(7)	0.450	667.76	
5-5		1f-1e		394.871(10)	0.367	669.29	
6-6		1f-1e		552.807(14)	0.310	671.13	
7-7		1f-1e		737.056(18)	0.268	673.27	
8-8		1f-1e		947.614(23)	0.236	675.71	
9-9		1f-1e		1 184.474(28)	0.211	678.47	
10-10		1f-1e		1 447.630(33)	0.191	681.53	
11-11		1f-1e		1 737.072(38)	0.174	684.89	
12-12		1f-1e		2 052.791(43)	0.160	688.56	
13-13		1f-1e		2 394.774(48)	0.148	692.54	
14-14		1f-1e		2 763.008(55)	0.138	696.82	
15-15		1f-1e		3 157.476(57)	0.129	701.41	
16-16		1f-1e		3 578.160(61)	0.121	706.31	
17-17		1f-1e		4 025.038(64)	0.114	711.51	
18-18		1f-1e		4 498.085(67)	0.108	717.01	

Table 12. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{13}\text{C}^{14}\text{N}$ in the $3v_7^{1/2}$ Vibrational State (Continued).

Transition J'-J''	F'-F''	l'-l''	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength	Energy Level of Lower State (cm^{-1})	Reference
19-19		1f-1e		4 997.273(69)	0.103	722.82	
20-20		1f-1e		5 522.571(70)	0.098	728.94	
21-21		1f-1e		6 073.942(71)	0.093	735.37	
22-22		1f-1e		6 651.346(70)	0.089	742.09	
23-23		1f-1e		7 254.738(68)	0.085	749.13	
24-24		1f-1e		7 884.068(66)	0.082	756.47	
25-25		1f-1e	8 539.04(10)	8 539.278(63)	0.078	764.12	68A
26-26		1f-1e	9 220.14(10)	9 220.307(59)	0.075	772.07	68A
27-27		1f-1e	9 927.14(10)	9 927.087(55)	0.073	780.33	68A
28-28		1f-1e	10 659.58(10)	10 659.541(50)	0.070	788.89	68A
29-29		1f-1e	11 417.71(10)	11 417.587(46)	0.068	797.76	68A
30-30		1f-1e	12 201.26(10)	12 201.133(42)	0.066	806.94	68A
31-31		1f-1e	13 010.16(10)	13 010.081(40)	0.064	816.42	68A
32-32		1f-1e	13 844.27(10)	13 844.321(39)	0.062	826.21	68A
33-33		1f-1e	14 703.91(10)	14 703.737(40)	0.060	836.30	68A
34-34		1f-1e	15 588.32(10)	15 588.202(43)	0.058	846.70	68A
35-35		1f-1e	16 497.62(10)	16 497.577(46)	0.056	857.40	68A
36-36		1f-1e	17 431.59(10)	17 431.715(49)	0.055	868.41	68A
37-37		1f-1e	18 390.43(10)	18 390.456(52)	0.053	879.73	68A
38-38		1f-1e	19 373.55(10)	19 373.628(54)	0.052	891.35	68A
39-39		1f-1e	20 381.01(10)	20 381.047(54)	0.051	903.27	68A
40-40		1f-1e	21 412.36(10)	21 412.518(55)	0.049	915.51	68A
41-41		1f-1e		22 467.831(57)	0.048	928.04	
42-42		1f-1e		23 546.763(65)	0.047	940.89	
43-43		1f-1e	24 649.07(10)	24 649.076(81)	0.046	954.04	77C
44-44		1f-1e	25 774.63(10)	25 774.52(11)	0.045	967.49	77C
45-45		1f-1e		26 922.83(15)	0.044	981.25	
46-46		1f-1e		28 093.72(20)	0.043	995.32	
47-47		1f-1e		29 286.89(26)	0.042	1009.69	
48-48		1f-1e		30 502.04(34)	0.041	1024.36	
49-49		1f-1e		31 738.84(43)	0.040	1039.34	
50-50		1f-1e		32 996.93(54)	0.040	1054.63	

^a Quadrupole hyperfine structure calculated assuming $eQq = -4.3188$ MHz. Uncertainties on the individual components should roughly follow the trend in Table 8.

^b Calculated from resolved components using $eQq = -4.3188$ MHz.

^c Lines used to calculate center frequency.

^d Blended line not used in least-squares fitting.

Table 13. Rotational Spectrum of $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ in the $3\nu_7^3$ Vibrational State

Transition J'-J''	F'-F''	Observed Frequency (Est. Uncertainty) in MHz	Calculated Frequency (Est. Uncertainty) in MHz	Line Strength ^a	Energy Level of Lower State (cm^{-1})	Reference
4-3		36 738.081(50) ^c	36 738.041(26) ^b	3.500	670.17	
	3-3		36 736.422	0.073		
	4-3	36 737.118(50) ^d	36 737.069	1.096		77B
	3-4		36 738.221	0.001		
	5-4	36 738.384(50) ^d	36 738.354	1.425		77B
	3-2		36 738.851	0.833		
	4-4		36 738.869	0.073		
5-4			45 922.481(30)	6.400	671.40	
	5-4		45 921.995	2.048		
	4-4		45 922.175	0.085		
	5-5		45 922.510	0.085		
	6-5		45 922.660	2.522		
	4-3		45 922.823	1.658		
6-5			55 106.873(33)	9.000	672.93	
	6-6		55 106.446	0.083		
	6-5		55 106.596	2.916		
	7-6		55 106.986	3.465		
	5-4		55 107.047	2.457		
	5-5		55 107.227	0.083		
7-6		64 291.08(10)	64 291.210(35)	11.429	674.77	77B
	7-7		64 290.496	0.078		
	7-6		64 291.036	3.737		
	8-7		64 291.286	4.320		
	6-5		64 291.308	3.223		
	6-6		64 291.939	0.078		
8-7		73 475.49(10)	73 475.480(35)	13.750	676.91	77B
	8-8		73 474.575	0.072		
	8-7		73 475.364	4.510		
	9-8		73 475.534	5.129		
	7-6		73 475.541	3.974		
	7-7		73 476.444	0.072		
9-8			82 659.675(35)	16.000	679.36	
10-9		91 843.79(10)	91 843.785(35)	18.200	682.12	77C
11-10			101 027.801(38)	20.364	685.18	
12-11			110 211.713(46)	22.500	688.55	
13-12		119 395.52(10)	119 395.512(61)	24.615	692.23	77C
14-13		128 579.20(20)	128 579.190(82)	26.714	696.21	77B
15-14			137 762.74(11)	28.800	700.50	

^a Each line is an unresolved doublet, therefore, the line strength for each transition has been multiplied by two.

^b Quadrupole hyperfine structure calculated assuming $eQq = -4.3188$ MHz.

^c Center frequency calculated from resolved components using $eQq = -4.3188$ MHz.

^d Lines used to calculate center frequency.

Table 14. Calculated Microwave Spectrum of HCCCN in Order of Frequency

Calculated Frequency (Est. Uncertainty) in MHz	Vib. State ^a	Transition J'-J''	Isotopic Species ^b	Calculated Frequency (Est. Uncertainty) in MHz	Vib. State ^a	Transition J'-J''	Isotopic Species ^b
5.162(16)	v ₅	1-1	1f-1f	737.056(18)	3v ₇	7-7	1f-1e
7.1770(85)	v ₆	1-1	1f-1e	751.82(44)	v ₆	14-14	1f-1e
13.0764(1)	v ₇	1-1	1f-1e	782.3(16)	v ₅	17-17	1f-1e
15.484(47)	v ₅	2-2	1f-1e	858.93(53)	v ₆	15-15	1f-1e
21.530(25)	v ₆	2-2	1f-1e	862.7711(41)	v ₇	11-11	1f-1e
26.326(1)	3v ₇	1-1	1f-1e	873.4(20)	v ₅	18-18	1f-1e
30.962(92)	v ₅	3-3	1f-1e	947.614(23)	3v ₇	8-8	1f-1e
39.2290(2)	v ₇	2-2	1f-1e	969.3(26)	v ₅	19-19	1f-1e
43.057(49)	v ₆	3-3	1f-1e	973.10(66)	v ₆	16-16	1f-1e
51.59(15)	v ₅	4-4	1f-1e	1 019.5707(40)	v ₇	12-12	1f-1e
71.756(79)	v ₆	4-4	1f-1e	1 069.9(33)	v ₅	20-20	1f-1e
77.36(22)	v ₅	5-5	1f-1e	1 094.31(86)	v ₆	17-17	1f-1e
78.4568(4)	v ₇	5-5	1f-1e	1 175.4(42)	v ₅	21-21	1f-1e
78.978(2)	3v ₇	2-2	1f-1e	1 184.474(28)	3v ₇	9-9	1f-1e
107.62(11)	v ₆	5-5	1f-1e	1 189.4329(56)	v ₇	13-13	1f-1e
108.27(29)	v ₅	6-6	1f-1e	1 222.6(11)	v ₆	18-18	1f-1e
130.7587(7)	v ₇	4-4	1f-1e	1 285.5(52)	v ₅	22-22	1f-1e
144.29(37)	v ₅	7-7	1f-1e	1 357.8(15)	v ₆	19-19	1f-1e
150.65(15)	v ₆	6-6	1f-1e	1 372.3286(64)	v ₇	14-14	1f-1e
157.953(4)	3v ₇	3-3	1f-1e	1 400.4(65)	v ₅	23-23	1f-1e
185.43(44)	v ₅	8-8	1f-1e	1 447.630(33)	3v ₇	10-10	1f-1e
196.1332(10)	v ₇	5-5	1f-1e	1 500.1(19)	v ₆	20-20	1f-1e
200.83(19)	v ₆	7-7	1f-1e	1 519.8(80)	v ₅	24-24	1f-1e
231.65(52)	v ₅	9-9	1f-1e	1 568.2604(72)	v ₇	15-15	1f-1e
258.17(23)	v ₆	8-8	1f-1e	1 643.9(96)	v ₅	25-25	1f-1e
263.252(7)	3v ₇	4-4	1f-1e	1 649.3(24)	v ₆	21-21	1f-1e
274.5785(14)	v ₇	6-6	1f-1e	1 737.072(38)	3v ₇	11-11	1f-1e
282.95(58)	v ₅	10-10	1f-1e	1 777.2227(81)	v ₇	16-16	1f-1e
322.65(27)	v ₆	9-9	1f-1e	1 805.5(30)	v ₆	22-22	1f-1e
336.0921(18)	v ₇	7-7	1f-1e	1 968.6(37)	v ₆	23-23	1f-1e
339.31(65)	v ₅	11-11	1f-1e	1 999.2093(89)	v ₇	17-17	1f-1e
394.26(30)	v ₆	10-10	1f-1e	2 052.791(43)	3v ₇	12-12	1f-1e
394.871(10)	3v ₇	5-5	1f-1e	2 138.6(45)	v ₆	24-24	1f-1e
400.71(71)	v ₅	12-12	1f-1e	2 234.2136(98)	v ₇	18-18	1f-1e
467.11(78)	v ₅	13-13	1f-1e	2 315.5(55)	v ₆	25-25	1f-1e
470.6715(23)	v ₇	8-8	1f-1e	2 394.774(48)	3v ₇	13-13	1f-1e
472.99(33)	v ₆	11-11	1f-1e	2 482.229(11)	v ₇	19-19	1f-1e
538.50(88)	v ₅	14-14	1f-1e	2 499.2(66)	v ₆	26-26	1f-1e
552.807(14)	3v ₇	6-6	1f-1e	2 689.8(78)	v ₆	27-27	1f-1e
558.83(35)	v ₆	12-12	1f-1e	2 743.247(12)	v ₇	20-20	1f-1e
588.3134(29)	v ₇	9-9	1f-1e	2 763.008(53)	3v ₇	14-14	1f-1e
614.9(10)	v ₅	15-15	1f-1e	2 887.2(92)	v ₆	28-28	1f-1e
651.78(39)	v ₆	13-13	1f-1e	3 017.262(13)	v ₇	21-21	1f-1e
696.1(13)	v ₅	16-16	1f-1e	3 157.476(57)	3v ₇	15-15	1f-1e
719.0146(35)	v ₇	10-10	1f-1e	3 304.265(14)	v ₇	22-22	1f-1e

Table 14. Calculated Microwave Spectrum of HCCCN in Order of Frequency (Continued)

Calculated Frequency (Est. Uncertainty) in MHz	Vib. State ^a	Transition		Isotopic Species ^b	Calculated Frequency (Est. Uncertainty) in MHz	Vib. State ^a	Transition		Isotopic Species ^b
		J'-J''	l'-l''				J'-J''	l'-l''	
3 578.160(61)	3v ₇	16-16	1f-1e		13 465.701(21)	v ₇	45-45	1f-1e	
3 604.246(15)	v ₇	23-23	1f-1e		13 844.321(39)	3v ₇	32-32	1f-1e	
3 917.199(15)	v ₇	24-24	1f-1e		14 060.997(20)	v ₇	46-46	1f-1e	
4 025.038(64)	3v ₇	17-17	1f-1e		14 668.955(20)	v ₇	47-47	1f-1e	
4 243.113(16)	v ₇	25-25	1f-1e		14 703.737(40)	3v ₇	33-33	1f-1e	
4 498.085(67)	3v ₇	18-18	1f-1e		15 289.557(20)	v ₇	48-48	1f-1e	
4 581.978(17)	v ₇	26-26	1f-1e		15 588.202(43)	3v ₇	34-34	1f-1e	
4 933.785(18)	v ₇	27-27	1f-1e		15 922.785(20)	v ₇	49-49	1f-1e	
4 997.273(69)	3v ₇	19-19	1f-1e		16 497.577(46)	3v ₇	35-35	1f-1e	
5 298.524(19)	v ₇	28-28	1f-1e		16 568.618(20)	v ₇	50-50	1f-1e	
5 522.571(70)	3v ₇	20-20	1f-1e		16 886.3122(17)		2- 1		2 12 12 12 14
5 676.184(20)	v ₇	29-29	1f-1e		17 227.040(21)	v ₇	51-51	1f-1e	
6 066.753(20)	v ₇	30-30	1f-1e		17 431.715(49)	3v ₇	36-36	1f-1e	
6 073.942(71)	3v ₇	21-21	1f-1e		17 633.7527(41)		2- 1		1 13 12 12 14
6 470.220(21)	v ₇	31-31	1f-1e		17 666.9948(38)		2- 1		1 12 12 12 15
6 651.346(70)	3v ₇	22-22	1f-1e		17 898.029(23)	v ₇	52-52	1f-1e	
6 886.573(22)	v ₇	32-32	1f-1e		18 119.0294(48)		2- 1		1 12 13 12 14
7 254.738(68)	3v ₇	23-23	1f-1e		18 120.7731(18)		2- 1		1 12 12 13 14
7 315.801(22)	v ₇	33-33	1f-1e		18 196.2183(5)		2- 1		
7 757.889(23)	v ₇	34-34	1f-1e		18 197.932(22)	v ₅	2- 1	1e-1e	
7 884.068(66)	3v ₇	24-24	1f-1e		18 208.254(22)	v ₅	2- 1	1f-1f	
8 212.826(23)	v ₇	35-35	1f-1e		18 226.036(12)	v ₆	2- 1	1e-1e	
8 443.1615(9)		1- 0		2 12 12 12 14	18 240.389(12)	v ₆	2- 1	1f-1f	
8 539.278(63)	3v ₇	25-25	1f-1e		18 240.9520(67)	v ₇	2- 1	1e-1e	
8 680.597(23)	v ₇	36-36	1f-1e		18 267.1045(67)	v ₇	2- 1	1f-1f	
8 816.8825(21)		1- 0		1 13 12 12 14	18 311.849(11)	2v ₇	2- 1	0 - 0	
8 833.5035(19)		1- 0		1 12 12 12 15	18 342.438(17)	3v ₇	2- 1	1e-1e	
9 059.5212(25)		1- 0		1 12 13 12 14	18 390.456(52)	3v ₇	37-37	1f-1e	
9 060.3930(9)		1- 0		1 12 12 13 14	18 395.090(17)	3v ₇	2- 1	1f-1f	
9 098.1157(3)		1- 0			18 581.566(25)	v ₇	53-53	1f-1e	
9 155.9391(55)	2v ₇	1- 0	0 - 0		19 277.630(27)	v ₇	54-54	1f-1e	
9 161.190(23)	v ₇	37-37	1f-1e		19 373.628(54)	3v ₇	38-38	1f-1e	
9 220.307(59)	3v ₇	26-26	1f-1e		19 986.201(31)	v ₇	55-55	1f-1e	
9 654.589(23)	v ₇	38-38	1f-1e		20 381.047(54)	3v ₇	39-39	1f-1e	
9 927.087(55)	3v ₇	27-27	1f-1e		20 707.258(35)	v ₇	56-56	1f-1e	
10 160.780(23)	v ₇	39-39	1f-1e		21 412.518(55)	3v ₇	40-40	1f-1e	
10 659.541(50)	3v ₇	28-28	1f-1e		21 440.779(39)	v ₇	57-57	1f-1e	
10 679.749(23)	v ₇	40-40	1f-1e		22 186.743(45)	v ₇	58-58	1f-1e	
11 211.480(23)	v ₇	41-41	1f-1e		22 467.831(57)	3v ₇	41-41	1f-1e	
11 417.587(46)	3v ₇	29-29	1f-1e		22 945.126(50)	v ₇	59-59	1f-1e	
11 755.956(22)	v ₇	42-42	1f-1e		23 546.763(65)	3v ₇	42-42	1f-1e	
12 201.133(42)	3v ₇	30-30	1f-1e		23 715.907(57)	v ₇	60-60	1f-1e	
12 313.163(22)	v ₇	43-43	1f-1e		24 649.076(81)	3v ₇	43-43	1f-1e	
12 883.084(22)	v ₇	44-44	1f-1e		25 329.4411(24)		3- 2		2 12 12 12 14
13 010.081(40)	3v ₇	31-31	1f-1e		25 774.52(11)	3v ₇	44-44	1f-1e	

Table 14. Calculated Microwave Spectrum of HCCCN in Order of Frequency (Continued)

Calculated Frequency (Est. Uncertainty) in MHz	Vib. State ^a	Transition		Isotopic Species ^b	Calculated Frequency (Est. Uncertainty) in MHz	Vib. State ^a	Transition		Isotopic Species ^b
		J'-J''	k'-k''				J'-J''	k'-k''	
26 450.5985(59)		3- 2		1 13 12 12 14	45 490.3161(12)		5- 4		
26 500.4616(54)		3- 2		1 12 12 12 15	45 494.540(47)	v ₅	5- 4	1e-1e	
26 922.83(15)	3v ₇	45-45	1f-1e		45 520.311(48)	v ₅	5- 4	1f-1f	
27 178.5115(69)		3- 2		1 12 13 12 14	45 564.872(24)	v ₆	5- 4	1e-1e	
27 181.1273(26)		3- 2		1 12 12 13 14	45 600.738(25)	v ₆	5- 4	1f-1f	
27 294.2947(8)		3- 2			45 602.145(16)	v ₇	5- 4	1e-1e	
27 296.857(32)	v ₅	3- 2	1e-1e		45 667.519(16)	v ₇	5- 4	1f-1f	
27 312.335(32)	v ₅	3- 2	1f-1f		45 778.864(28)	2v ₇	5- 4	2e-2e	
27 339.023(17)	v ₆	3- 2	1e-1e		45 779.105(26)	2v ₇	5- 4	0 - 0	
27 360.550(17)	v ₆	3- 2	1f-1f		45 779.167(28)	2v ₇	5- 4	2f-2f	
27 361.3944(100)	v ₇	3- 2	1e-1e		45 855.853(36)	3v ₇	5- 4	1e-1e	
27 400.6222(100)	v ₇	3- 2	1f-1f		45 922.481(30)	3v ₇	5- 4	3 - 3	
27 467.433(17)	2v ₇	3- 2	2e-2e		45 987.472(36)	3v ₇	5- 4	1f-1f	
27 467.494(17)	2v ₇	3- 2	2f-2f		50 658.5887(40)		6- 5		2 12 12 12 14
27 467.699(16)	2v ₇	3- 2	0 - 0		52 900.8672(90)		6- 5		1 13 12 12 14
27 513.623(24)	3v ₇	3- 2	1e-1e		53 000.5926(85)		6- 5		1 12 12 12 15
27 592.599(24)	3v ₇	3- 2	1f-1f		54 356.671(11)		6- 5		1 12 13 12 14
28 093.72(20)	3v ₇	46-46	1f-1e		54 361.9045(44)		6- 5		1 12 12 13 14
29 286.89(26)	3v ₇	47-47	1f-1e		54 588.2351(14)		6- 5		
30 502.04(34)	3v ₇	48-48	1f-1e		54 593.265(51)	v ₅	6- 5	1e-1e	
31 738.84(43)	3v ₇	49-49	1f-1e		54 624.170(53)	v ₅	6- 5	1f-1f	
32 996.93(54)	3v ₇	50-50	1f-1e		54 677.710(27)	v ₆	6- 5	1e-1e	
33 772.5374(31)		4- 3		2 12 12 12 14	54 720.738(28)	v ₆	6- 5	1f-1f	
35 267.4077(73)		4- 3		1 13 12 12 14	54 722.425(19)	v ₇	6- 5	1e-1e	
35 333.8917(68)		4- 3		1 12 12 12 15	54 800.871(19)	v ₇	6- 5	1f-1f	
36 237.9544(87)		4- 3		1 12 13 12 14	54 934.478(33)	2v ₇	6- 5	2e-2e	
36 241.4425(33)		4- 3		1 12 12 13 14	54 934.602(30)	2v ₇	6- 5	0 - 0	
36 392.3316(10)		4- 3			54 935.009(32)	2v ₇	6- 5	2f-2f	
36 395.732(40)	v ₅	4- 3	1e-1e		55 026.872(39)	3v ₇	6- 5	1e-1e	
36 416.360(41)	v ₅	4- 3	1f-1f		55 106.873(33)	3v ₇	6- 5	3 - 3	
36 451.973(21)	v ₆	4- 3	1e-1e		55 184.808(39)	3v ₇	6- 5	1f-1f	
36 480.671(22)	v ₆	4- 3	1f-1f		59 101.5220(42)		7- 6		2 12 12 12 14
36 481.796(13)	v ₇	4- 3	1e-1e		61 717.4931(93)		7- 6		1 13 12 12 14
36 534.098(13)	v ₇	4- 3	1f-1f		61 833.8390(88)		7- 6		1 12 12 12 15
36 623.177(23)	2v ₇	4- 3	2e-2e		63 415.918(11)		7- 6		1 12 13 12 14
36 623.329(23)	2v ₇	4- 3	2f-2f		63 422.0253(48)		7- 6		1 12 12 13 14
36 623.461(21)	2v ₇	4- 3	0 - 0		63 686.0753(15)		7- 6		
36 684.766(31)	3v ₇	4- 3	1e-1e		63 691.891(54)	v ₅	7- 6	1e-1e	
36 738.041(26)	3v ₇	4- 3	3 - 3		63 727.917(56)	v ₅	7- 6	1f-1f	
36 790.064(31)	3v ₇	4- 3	1f-1f		63 790.472(28)	v ₆	7- 6	1e-1e	
42 215.5902(36)		5- 4		2 12 12 12 14	63 840.657(29)	v ₆	7- 6	1f-1f	
44 084.1680(84)		5- 4		1 13 12 12 14	63 842.625(21)	v ₇	7- 6	1e-1e	
44 167.2728(78)		5- 4		1 12 12 12 15	63 934.139(21)	v ₇	7- 6	1f-1f	
45 297.345(10)		5- 4		1 12 13 12 14	64 089.921(34)	2v ₇	7- 6	0 - 0	
45 301.7059(39)		5- 4		1 12 12 13 14	64 090.007(38)	2v ₇	7- 6	2e-2e	

Table 14. Calculated Microwave Spectrum of HCCCN in Order of Frequency (Continued)

Calculated Frequency (Est. Uncertainty) in MHz	Vib. State ^a	Transition		Isotopic Species ^b	Calculated Frequency (Est. Uncertainty) in MHz	Vib. State ^a	Transition		Isotopic Species ^b
		J'-J''	K'-K''				J'-J''	K'-K''	
64 090.855(36)	2v ₇	7- 6	2f-2f		90 978.9933(21)		10- 9		
64 197.807(41)	3v ₇	7- 6	1e-1e		90 987.005(58)	v ₅	10- 9	1e-1e	
64 291.210(35)	3v ₇	7- 6	3 -3		91 038.307(61)	v ₅	10- 9	1f-1f	
64 382.057(41)	3v ₇	7- 6	1f-1f		91 128.186(28)	v ₆	10- 9	1e-1e	
67 544.3792(43)		8- 7		2 12 12 12 14	91 199.796(32)	v ₆	10- 9	1f-1f	
70 534.0334(92)		8- 7		1 13 12 12 14	91 202.607(27)	v ₇	10- 9	1e-1e	
70 666.9996(89)		8- 7		1 12 12 12 15	91 333.308(27)	v ₇	10- 9	1f-1f	
72 475.074(11)		8- 7		1 12 13 12 14	91 554.521(43)	2v ₇	10- 9	0 -0	
72 482.0553(51)		8- 7		1 12 12 13 14	91 555.932(49)	2v ₇	10- 9	2e-2e	
72 783.8238(17)		8- 7			91 558.432(45)	2v ₇	10- 9	2f-2f	
72 790.401(55)	v ₅	8- 7	1e-1e		91 709.980(55)	3v ₇	10- 9	1e-1e	
72 831.535(58)	v ₅	8- 7	1f-1f		91 843.785(35)	3v ₇	10- 9	3 -3	
72 903.147(28)	v ₆	8- 7	1e-1e		91 973.135(55)	3v ₇	10- 9	1f-1f	
72 960.482(29)	v ₆	8- 7	1f-1f		92 872.3861(44)		11-10		2 12 12 12 14
72 962.731(24)	v ₇	8- 7	1e-1e		96 983.0177(92)		11-10		1 13 12 12 14
73 067.311(24)	v ₇	8- 7	1f-1f		97 165.8433(93)		11-10		1 12 12 12 15
73 245.034(38)	2v ₇	8- 7	0 -0		99 651.863(12)		11-10		1 12 13 12 14
73 245.435(42)	2v ₇	8- 7	2e-2e		99 661.4707(64)		11-10		1 12 12 13 14
73 246.708(40)	2v ₇	8- 7	2f-2f		100 076.3883(23)		11-10		
73 368.646(44)	3v ₇	8- 7	1e-1e		100 085.067(66)	v ₅	11-10	1e-1e	
73 475.480(35)	3v ₇	8- 7	3 -3		100 141.425(69)	v ₅	11-10	1f-1f	
73 579.204(44)	3v ₇	8- 7	1f-1f		100 240.524(31)	v ₆	11-10	1e-1e	
75 987.1496(43)		9- 8		2 12 12 12 14	100 319.258(38)	v ₆	11-10	1f-1f	
79 350.4757(90)		9- 8		1 13 12 12 14	100 322.349(29)	v ₇	11-10	1e-1e	
79 500.0620(88)		9- 8		1 12 12 12 15	100 466.106(29)	v ₇	11-10	1f-1f	
81 534.125(11)		9- 8		1 12 13 12 14	100 708.837(45)	2v ₇	11-10	0 -0	
81 541.9815(54)		9- 8		1 12 12 13 14	100 710.972(52)	2v ₇	11-10	2e-2e	
81 881.4675(19)		9- 8			100 714.306(47)	2v ₇	11-10	2f-2f	
81 888.778(56)	v ₅	9- 8	1e-1e		100 880.448(70)	3v ₇	11-10	1e-1e	
81 935.004(59)	v ₅	9- 8	1f-1f		101 027.801(38)	3v ₇	11-10	3 -3	
82 015.723(27)	v ₆	9- 8	1e-1e		101 169.890(70)	3v ₇	11-10	1f-1f	
82 080.199(29)	v ₆	9- 8	1f-1f		101 314.8307(47)		12-11		2 12 12 12 14
82 082.730(26)	v ₇	9- 8	1e-1e		105 799.093(10)		12-11		1 13 12 12 14
82 200.372(26)	v ₇	9- 8	1f-1f		105 998.537(10)		12-11		1 12 12 12 15
82 399.910(41)	2v ₇	9- 8	0 -0		108 710.523(12)		12-11		1 12 13 12 14
82 400.748(46)	2v ₇	9- 8	2e-2e		108 721.0077(72)		12-11		1 12 12 13 14
82 402.566(43)	2v ₇	9- 8	2f-2f		109 173.6394(25)		12-11		
82 539.375(47)	3v ₇	9- 8	1e-1e		109 182.946(81)	v ₅	12-11	1e-1e	
82 659.675(35)	3v ₇	9- 8	3 -3		109 244.339(84)	v ₅	12-11	1f-1f	
82 776.235(47)	3v ₇	9- 8	1f-1f		109 352.726(39)	v ₆	12-11	1e-1e	
84 429.8221(43)		10- 9		2 12 12 12 14	109 438.572(49)	v ₆	12-11	1f-1f	
88 166.8080(89)		10- 9		1 13 12 12 14	109 441.944(30)	v ₇	12-11	1e-1e	
88 333.0141(89)		10- 9		1 12 12 12 15	109 598.751(30)	v ₇	12-11	1f-1f	
90 593.059(11)		10- 9		1 12 13 12 14	109 757.1450(54)		13-12		2 12 12 12 14
90 601.7910(58)		10- 9		1 12 12 13 14	109 862.828(46)	2v ₇	12-11	0 -0	

Table 14. Calculated Microwave Spectrum of HCCCN in Order of Frequency (Continued)

Calculated Frequency (Est. Uncertainty) in MHz	Vib. State ^a	Transition J'-J'' & l'-l''	Isotopic Species ^b	Calculated Frequency (Est. Uncertainty) in MHz	Vib. State ^a	Transition J'-J'' & l'-l''	Isotopic Species ^b
109 865.854(55)	2v ₇	12-11 2e-2e		135 898.632(10)		15-14	1 12 12 13 14
109 870.188(48)	2v ₇	12-11 2f-2f		136 464.3999(23)		15-14	
110 050.765(92)	3v ₇	12-11 1e-1e		136 475.32(19)	v ₅	15-14 1e-1e	
110 211.713(46)	3v ₇	12-11 3-3		136 551.67(19)	v ₅	15-14 1f-1f	
110 366.484(92)	3v ₇	12-11 1f-1f		136 688.382(95)	v ₆	15-14 1e-1e	
114 615.021(12)		13-12	1 13 12 12 14	136 795.492(115)	v ₆	15-14 1f-1f	
114 831.084(11)		13-12	1 12 12 12 15	136 799.704(31)	v ₇	15-14 1e-1e	
117 769.027(14)		13-12	1 12 13 12 14	136 995.636(31)	v ₇	15-14 1f-1f	
117 780.3890(81)		13-12	1 12 12 13 14	137 322.558(48)	2v ₇	15-14 0-0	
118 199.5185(63)		14-13	2 12 12 12 14	137 329.410(59)	2v ₇	15-14 2e-2e	
118 270.7336(26)		13-12		137 337.896(50)	2v ₇	15-14 2f-2f	
118 280.63(11)	v ₅	13-12 1e-1e		137 560.68(21)	3v ₇	15-14 1e-1e	
118 347.03(11)	v ₅	13-12 1f-1f		137 762.74(11)	3v ₇	15-14 3-3	
118 464.777(53)	v ₆	13-12 1e-1e		137 955.15(21)	3v ₇	15-14 1f-1f	
118 557.724(66)	v ₆	13-12 1f-1f		141 061.797(15)		16-15	1 13 12 12 14
118 561.376(30)	v ₇	13-12 1e-1e		141 327.714(14)		16-15	1 12 12 12 15
118 731.231(30)	v ₇	13-12 1f-1f		143 524.8839(98)		17-16	2 12 12 12 14
119 016.465(47)	2v ₇	13-12 0-0		144 943.469(16)		16-15	1 12 13 12 14
119 020.564(56)	2v ₇	13-12 2e-2e		144 957.468(11)		16-15	1 12 12 13 14
119 026.080(49)	2v ₇	13-12 2f-2f		145 560.9462(19)		16-15	
119 220.92(12)	3v ₇	13-12 1e-1e		145 572.30(24)	v ₅	16-15 1e-1e	
119 395.512(61)	3v ₇	13-12 3-3		145 653.59(24)	v ₅	16-15 1f-1f	
119 562.90(12)	3v ₇	13-12 1f-1f		145 799.91(12)	v ₆	16-15 1e-1e	
123 430.789(13)		14-13	1 13 12 12 14	145 914.08(15)	v ₆	16-15 1f-1f	
123 663.471(12)		14-13	1 12 12 12 15	145 918.572(31)	v ₇	16-15 1e-1e	
126 641.3397(74)		15-14	2 12 12 12 14	146 127.534(31)	v ₇	16-15 1f-1f	
126 827.361(15)		14-13	1 12 13 12 14	146 474.956(49)	2v ₇	16-15 0-0	
126 839.6015(92)		14-13	1 12 12 13 14	146 483.516(60)	2v ₇	16-15 2e-2e	
127 367.6581(25)		14-13		146 493.821(51)	2v ₇	16-15 2f-2f	
127 378.09(14)	v ₅	14-13 1e-1e		146 730.27(26)	3v ₇	16-15 1e-1e	
127 449.48(14)	v ₅	14-13 1f-1f		147 150.95(26)	3v ₇	16-15 1f-1f	
127 576.667(71)	v ₆	14-13 1e-1e		149 877.013(16)		17-16	1 13 12 12 14
127 676.703(88)	v ₆	14-13 1f-1f		150 159.546(14)		17-16	1 12 12 12 15
127 680.634(31)	v ₇	14-13 1e-1e		151 966.385(11)		18-17	2 12 12 12 14
127 863.530(31)	v ₇	14-13 1f-1f		154 001.217(16)		17-16	1 12 13 12 14
128 169.718(48)	2v ₇	14-13 0-0		154 016.096(12)		17-16	1 12 12 13 14
128 175.088(58)	2v ₇	14-13 2e-2e		154 657.2840(16)		17-16	
128 181.982(49)	2v ₇	14-13 2f-2f		154 669.02(30)	v ₅	17-16 1e-1e	
128 390.90(16)	3v ₇	14-13 1e-1e		154 755.20(30)	v ₅	17-16 1f-1f	
128 579.190(82)	3v ₇	14-13 3-3		154 911.24(16)	v ₆	17-16 1e-1e	
128 759.13(16)	3v ₇	14-13 1f-1f		155 032.45(19)	v ₆	17-16 1f-1f	
132 246.385(14)		15-14	1 13 12 12 14	155 037.224(31)	v ₇	17-16 1e-1e	
132 495.685(13)		15-14	1 12 12 12 15	155 259.210(31)	v ₇	17-16 1f-1f	
135 083.1985(86)		16-15	2 12 12 12 14	155 626.881(51)	2v ₇	17-16 0-0	
135 885.513(16)		15-14	1 12 13 12 14	155 637.393(61)	2v ₇	17-16 2e-2e	

Table 14. Calculated Microwave Spectrum of HCCCN in Order of Frequency (Continued)

Calculated Frequency (Est. Uncertainty) in MHz	Vib. State ^a	Transition J'-J'' l'-l''	Isotopic Species ^b	Calculated Frequency (Est. Uncertainty) in MHz	Vib. State ^a	Transition J'-J'' l'-l''	Isotopic Species ^b
155 649.759(53)	2v ₇	17-16	2f-2f	182 243.90(29)	v ₆	20-19	1e-1e
155 899.64(32)	3v ₇	17-16	1e-1e	182 386.15(34)	v ₆	20-19	1f-1f
156 346.52(32)	3v ₇	17-16	1f-1f	182 391.754(35)	v ₇	20-19	1e-1e
158 692.019(19)		18-17	1 13 12 12 14	182 652.775(35)	v ₇	20-19	1f-1f
158 991.168(15)		18-17	1 12 12 12 15	183 079.527(68)	2v ₇	20-19	0 -0
160 407.691(12)		19-18	2 12 12 12 14	183 097.502(65)	2v ₇	20-19	2e-2e
163 058.743(16)		18-17	1 12 13 12 14	183 117.656(73)	2v ₇	20-19	2f-2f
163 074.504(13)		18-17	1 12 12 13 14	183 406.33(57)	3v ₇	20-19	1e-1e
163 753.4007(24)		18-17		183 931.63(57)	3v ₇	20-19	1f-1f
163 765.46(37)	v ₅	18-17	1e-1e	185 135.656(56)		21-20	1 13 12 12 14
163 856.51(38)	v ₅	18-17	1f-1f	185 484.646(43)		21-20	1 12 12 12 15
164 022.35(20)	v ₆	18-17	1e-1e	185 730.333(11)		22-21	2 12 12 12 14
164 150.60(23)	v ₆	18-17	1f-1f	190 229.863(47)		21 20	1 12 13 12 14
164 155.647(32)	v ₇	18-17	1e-1e	190 248.270(16)		21-20	1 12 12 13 14
164 390.652(32)	v ₇	18-17	1f-1f	191 040.296(13)		21-20	
164 778.304(55)	2v ₇	18-17	0 -0	191 052.90(66)	v ₅	21-20	1e-1e
164 791.026(63)	2v ₇	18-17	2e-2e	191 158.34(66)	v ₅	21-20	1f-1f
164 805.710(57)	2v ₇	18-17	2f-2f	191 354.31(34)	v ₆	21-20	1e-1e
165 068.78(40)	3v ₇	18-17	1e-1e	191 503.53(40)	v ₆	21-20	1f-1f
165 541.83(40)	3v ₇	18-17	1f-1f	191 509.410(38)	v ₇	21-20	1e-1e
167 506.803(26)		19-18	1 13 12 12 14	191 783.425(38)	v ₇	21-20	1f-1f
167 822.567(19)		19-18	1 12 12 12 15	192 229.268(79)	2v ₇	21-20	0 -0
168 848.792(12)		20-19	2 12 12 12 14	192 250.316(73)	2v ₇	21-20	2e-2e
172 116.035(19)		19-18	1 12 13 12 14	192 273.652(85)	2v ₇	21-20	2f-2f
172 132.677(14)		19-18	1 12 12 13 14	192 574.72(67)	3v ₇	21-20	1e-1e
172 849.2834(47)		19-18		193 126.09(67)	3v ₇	21-20	1f-1f
172 861.59(46)	v ₅	19-18	1e-1e	193 949.699(82)		22-21	1 13 12 12 14
172 957.48(46)	v ₅	19-18	1f-1f	194 170.7527(95)		23-22	2 12 12 12 14
173 133.25(24)	v ₆	19-18	1e-1e	194 315.302(64)		22-21	1 12 12 12 15
173 268.50(28)	v ₆	19-18	1f-1f	199 286.373(72)		22-21	1 12 13 12 14
173 273.828(33)	v ₇	19-18	1e-1e	199 305.663(18)		22-21	1 12 12 13 14
173 521.844(33)	v ₇	19-18	1f-1f	200 135.401(19)		22-21	
173 929.196(60)	2v ₇	19-18	0 -0	200 148.04(77)	v ₅	22-21	1e-1e
173 944.400(65)	2v ₇	19-18	2e-2e	200 258.20(77)	v ₅	22-21	1f-1f
173 961.676(63)	2v ₇	19-18	2f-2f	200 464.45(41)	v ₆	22-21	1e-1e
174 237.68(48)	3v ₇	19-18	1e-1e	200 620.62(47)	v ₆	22-21	1f-1f
174 736.87(48)	3v ₇	19-18	1f-1f	200 626.784(43)	v ₇	22-21	1e-1e
176 321.353(38)		20-19	1 13 12 12 14	200 913.786(43)	v ₇	22-21	1f-1f
176 653.731(28)		20-19	1 12 12 12 15	201 378.389(93)	2v ₇	22-21	0 -0
177 289.676(12)		21-20	2 12 12 12 14	201 402.828(80)	2v ₇	22-21	2e-2e
181 173.079(29)		20-19	1 12 13 12 14	201 429.665(101)	2v ₇	22-21	2f-2f
181 190.603(14)		20-19	1 12 12 13 14	201 742.82(79)	3v ₇	22-21	1e-1e
181 944.9194(81)		20-19		202 320.23(79)	3v ₇	22-21	1f-1f
181 957.41(55)	v ₅	20-19	1e-1e	202 610.9236(86)		24-23	2 12 12 12 14
182 058.09(55)	v ₅	20-19	1f-1f	202 763.47(12)		23-22	1 13 12 12 14

Table 14. Calculated Microwave Spectrum of HCCCN in Order of Frequency (Continued)

Calculated Frequency (Est. Uncertainty) in MHz	Vib. State ^a	Transition J'-J'' ℓ'-ℓ''	Isotopic Species ^b	Calculated Frequency (Est. Uncertainty) in MHz	Vib. State ^a	Transition J'-J'' ℓ'-ℓ''	Isotopic Species ^b
203 145.683(92)		23-22	1 12 12 12 15	228 821.74(15)	2v ₇	25-24	0 -0
208 342.60(11)		23-22	1 12 13 12 14	228 858.41(11)	2v ₇	25-24	2e-2e
208 362.770(24)		23-22	1 12 12 13 14	228 897.81(16)	2v ₇	25-24	2f-2f
209 230.221(26)		23-22		229 203.02(28)		26-25	1 13 12 12 14
209 242.82(90)	v ₅	23-22	1e-1f	229 245.4(12)	3v ₇	25-24	1e-1e
209 357.65(90)	v ₅	23-22	1f-1f	229 635.06(23)		26-25	1 12 12 12 15
209 574.32(47)	v ₆	23-22	1e-1e	229 900.6(12)	3v ₇	25-24	1f-1f
209 737.42(55)	v ₆	23-22	1f-1f	235 509.42(27)		26-25	1 12 13 12 14
209 743.861(50)	v ₇	23-22	1e-1e	235 532.241(59)		26-25	1 12 12 13 14
210 043.843(50)	v ₇	23-22	1f-1f	236 368.910(37)		28-27	2 12 12 12 14
210 526.860(109)	2v ₇	23-22	0 -0	236 512.849(62)		26-25	
210 555.025(89)	2v ₇	23-22	2e-2e	236 524.8(14)	v ₅	26-25	1e-1e
210 858.696(119)	2v ₇	23-22	2f-2f	236 653.4(14)	v ₅	26-25	1f-1f
210 910.65(91)	3v ₇	23-22	1e-1e	236 902.16(72)	v ₆	26-25	1e-1e
211 050.835(10)		25-24	2 12 12 12 14	237 085.91(83)	v ₆	26-25	1f-1f
211 514.04(91)	3v ₇	23-22	1f-1f	237 093.183(79)	v ₇	26-25	1e-1e
211 576.96(16)		24-23	1 13 12 12 14	237 432.049(79)	v ₇	26-25	1f-1f
211 975.78(13)		24-23	1 12 12 12 15	237 968.08(17)	2v ₇	26-25	0 -0
217 398.52(15)		24-23	1 12 13 12 14	238 009.57(13)	2v ₇	26-25	2e-2e
217 419.577(32)		24-23	1 12 12 13 14	238 015.57(36)		27-26	1 13 12 12 14
218 324.744(36)		24-23		238 053.90(19)	2v ₇	26-25	2f-2f
218 337.2(10)	v ₅	24-23	1e-1e	238 412.3(14)	3v ₇	26-25	1e-1e
218 456.7(10)	v ₅	24-23	1f-1f	238 464.22(30)		27-26	1 12 12 12 15
218 683.90(55)	v ₆	24-23	1e-1e	239 093.3(14)	3v ₇	26-25	1f-1f
218 853.91(63)	v ₆	24-23	1f-1f	244 564.37(36)		27-26	1 12 13 12 14
218 860.629(58)	v ₇	24-23	1e-1e	244 588.071(79)		27-26	1 12 12 13 14
219 173.582(58)	v ₇	24-23	1f-1f	244 807.679(52)		29-28	2 12 12 12 14
219 490.477(16)		26-25	2 12 12 12 14	245 606.406(79)		27-26	
219 674.65(13)	2v ₇	24-23	0 -0	245 617.9(15)	v ₅	27-26	1e-1e
219 706.89(10)	2v ₇	24-23	2e-2e	245 751.0(15)	v ₅	27-26	1f-1f
219 741.74(14)	2v ₇	24-23	2f-2f	246 010.80(82)	v ₆	27-26	1e-1e
220 078.2(10)	3v ₇	24-23	1e-1e	246 201.40(94)	v ₆	27-26	1f-1f
220 390.14(21)		25-24	1 13 12 12 14	246 208.942(91)	v ₇	27-26	1e-1e
220 707.5(10)	3v ₇	24-23	1f-1f	246 560.749(91)	v ₇	27-26	1f-1f
220 805.57(17)		25-24	1 12 12 12 15	246 827.79(46)		28-27	1 13 12 12 14
226 454.13(21)		25-24	1 12 13 12 14	247 113.66(20)	2v ₇	27-26	0 -0
226 476.072(44)		25-24	1 12 12 13 14	247 160.36(15)	2v ₇	27-26	2e-2e
227 418.957(47)		25-24		247 210.01(22)	2v ₇	27-26	2f-2f
227 431.2(12)	v ₅	25-24	1e-1e	247 293.04(38)		28-27	1 12 12 12 15
227 555.3(12)	v ₅	25-24	1f-1f	247 578.8(15)	3v ₇	27-26	1e-1e
227 793.19(63)	v ₆	25-24	1e-1e	248 285.6(15)	3v ₇	27-26	1f-1f
227 929.839(25)		27-26	2 12 12 12 14	253 246.136(71)		30-29	2 12 12 12 14
227 970.08(73)	v ₆	25-24	1f-1f	253 618.97(46)		28-27	1 12 13 12 14
227 977.074(68)	v ₇	25-24	1e-1e	253 643.55(10)		28-27	1 12 12 13 14
228 302.988(68)	v ₇	25-24	1f-1f	254 699.617(99)		28-27	

Table 14. Calculated Microwave Spectrum of HCCCN in Order of Frequency (Continued)

Calculated Frequency (Est. Uncertainty) in MHz	Vib. State ^a	Transition J'-J''	Isotopic Species ^b	Calculated Frequency (Est. Uncertainty) in MHz	Vib. State ^a	Transition J'-J''	Isotopic Species ^b
254 710.6(17)	v ₅	28-27	1e-1e	275 076.4(22)	3v ₇	30-29	1e-1e
254 848.1(17)	v ₅	28-27	1f-1f	275 859.9(22)	3v ₇	30-29	1f-1f
255 119.11(92)	v ₆	28-27	1e-1e	278 559.53(16)		33-32	2 12 12 12 14
255 316.52(105)	v ₆	28-27	1f-1f	280 780.53(89)		31-30	1 12 13 12 14
255 324.34(11)	v ₇	28-27	1e-1e	280 807.74(21)		31-30	1 12 12 13 14
255 639.66(58)		29-28	1 13 12 12 14	281 977.05(18)		31-30	
255 689.08(11)	v ₇	28-27	1f-1f	281 985.9(24)	v ₅	31-30	1e-1e
256 121.51(48)		29-28	1 12 12 12 15	282 073.0(11)		32-31	1 13 12 12 14
256 258.45(23)	2v ₇	28-27	0 -0	282 136.4(24)	v ₅	31-30	1f-1f
256 310.77(17)	2v ₇	28-27	2e-2e	282 441.9(13)	v ₆	31-30	1e-1e
256 366.14(25)	2v ₇	28-27	2f-2f	282 604.67(89)		32-31	1 12 12 12 15
256 745.0(17)	3v ₇	28-27	1e-1e	282 659.6(15)	v ₆	31-30	1f-1f
257 477.5(17)	3v ₇	28-27	1f-1f	282 668.21(16)	v ₇	31-30	1e-1e
261 684.270(95)		31-30	2 12 12 12 14	283 071.67(16)	v ₇	31-30	1f-1f
262 673.20(58)		29-28	1 12 13 12 14	283 687.71(34)	2v ₇	31-30	0 -0
262 698.66(13)		29-28	1 12 12 13 14	283 759.50(25)	2v ₇	31-30	2e-2e
263 792.47(12)		29-28		283 834.66(37)	2v ₇	31-30	2f-2f
263 802.9(20)	v ₅	29-28	1e-1e	284 241.5(24)	3v ₇	31-30	1e-1e
263 944.8(20)	v ₅	29-28	1f-1f	285 050.5(24)	3v ₇	31-30	1f-1f
264 277.1(10)	v ₆	29-28	1e-1e	286 996.63(19)		34-33	2 12 12 12 14
264 431.3(12)	v ₆	29-28	1f-1f	289 833.6(11)		32-31	1 12 13 12 14
264 439.36(12)	v ₇	29-28	1e-1e	289 861.68(26)		32-31	1 12 12 13 14
264 451.17(72)		30-29	1 13 12 12 14	290 883.4(13)		33-32	1 13 12 12 14
264 817.01(12)	v ₇	29-28	1f-1f	291 068.75(22)		32-31	
264 949.61(60)		30-29	1 12 12 12 15	291 076.6(27)	v ₅	32-31	1e-1e
265 402.40(26)	2v ₇	29-28	0 -0	291 231.3(27)	v ₅	32-31	1f-1f
265 460.76(19)	2v ₇	29-28	2e-2e	291 431.6(11)		33-32	1 12 12 12 15
265 522.29(29)	2v ₇	29-28	2f-2f	291 548.7(14)	v ₆	32-31	1e-1f
265 910.9(19)	3v ₇	29-28	1e-1e	291 773.1(16)	v ₆	32-31	1f-1f
266 668.9(19)	3v ₇	29-28	1f-1f	291 782.01(18)	v ₇	32-31	1e-1e
270 122.07(12)		32-31	2 12 12 12 14	292 198.37(18)	v ₇	32-31	1f-1f
271 727.06(72)		30-29	1 12 13 12 14	292 829.01(38)	2v ₇	32-31	0 -0
271 753.40(17)		30-29	1 12 12 13 14	292 908.21(28)	2v ₇	32-31	2e-2e
272 884.95(15)		30-29		292 990.88(42)	2v ₇	32-31	2f-2f
272 894.6(22)	v ₅	30-29	1e-1e	293 406.3(26)	3v ₇	32-31	1e-1e
273 040.8(22)	v ₅	30-29	1f-1f	294 240.5(26)	3v ₇	32-31	1f-1f
273 262.30(88)		31-30	1 13 12 12 14	295 433.37(24)		35-34	2 12 12 12 14
273 334.7(12)	v ₆	30-29	1e-1e	298 886.2(13)		33-32	1 12 13 12 14
273 545.6(13)	v ₆	30-29	1f-1f	298 915.20(31)		33-32	1 12 12 13 14
273 553.98(14)	v ₇	30-29	1e-1e	300 160.05(26)		33-32	
273 777.33(73)		31-30	1 12 12 12 15	301 969.37(42)	2v ₇	33-32	0 -0
273 944.55(14)	v ₇	30-29	1f-1f	302 056.45(31)	2v ₇	33-32	2e-2e
274 545.50(30)	2v ₇	30-29	0 -0	302 147.13(47)	2v ₇	33-32	2f-2f
274 610.35(22)	2v ₇	30-29	2e-2e				
274 678.46(33)	2v ₇	30-29	2f-2f				

^a No notation in this column indicates the ground vibrational state.

^b No notation in this column indicates the $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ isotopic species. The numbers given in the column refer to the atomic number of the atoms in the order HCCCN.

3.1. HCCCN References

a. Laboratory Literature References

- [50A] A. A. Westenberg and E. B. Wilson, Jr., *J. Am. Chem. Soc.* **72**, 199 (1950). "The Microwave Spectrum and Molecular Structure of Cyanoacetylene."
- [58A] C. C. Costain, *J. Chem. Phys.* **29**, 864 (1958). "Determination of Molecular Structures from Ground State Rotational Constants."
- [63A] J. K. Tyler and J. Sheridan, *Trans. Faraday Soc.* **59**, 2661 (1963). "Structural Studies of Linear Molecules by Microwave Spectroscopy."
- [68A] W. J. Lafferty, *J. Mol. Spectrosc.* **25**, 359 (1968). "Direct l -type Doubling Transitions in Some Axially Symmetric Molecules."
- [71A] D. R. Johnson and F. J. Lovas, *Astrophys. J.* **169**, 617 (1971). "A New Look at the Laboratory Microwave Spectrum of Cyanoacetylene."
- [71B] R. L. DeZafra, *Astrophys. J.* **170**, 165 (1971). "Precise Laboratory Determination of Rotational Transition Frequencies in Cyanoacetylene."
- [76A] See Section 3.1.b, Churchwell et al. (1977).
- [77A] R. A. Creswell, G. Winniewisser, and M.C. L. Gerry, *J. Mol. Spectrosc.* **65**, 420 (1977). "Rotational Spectra of the ^{13}C and ^{15}N Isotopic Species of Cyanoacetylene."
- [77B] P. D. Mallinson and R. L. DeZafra, *Mol. Phys.* to be published. "The Microwave Spectrum of Cyanoacetylene in Ground and Excited Vibrational States."
- [77C] Present work.

b. Astronomical Literature References

- B. E. Truner, *Astrophys. J. (Letters)* **163**, L35 (1971). "Detection of Interstellar Cyanoacetylene."
- D. F. Dickinson, *Astrophys. Lett.* **12**, 235 (1972). "Detection of Cyanoacetylene at 18 GHz."
- R. X. McGee, L. M. Newton, R. A. Batchelor and A. R. Kerr, *Astrophys. Lett.* **13**, 25 (1973). "The Cyanoacetylene Cloud in Sagittarius B2."
- P. M. Solomon, A. A. Penzias, K. B. Jefferts, and R. W. Wilson, *Astrophys. J. (Letters)* **185**, L63 (1973). "Millimeter Emission Lines of Polyatomic Molecules in Sagittarius B2."
- F. F. Gardner and G. Winniewisser, *Astrophys. J. (Letters)* **197**, L73 (1975). "Observations of the $J=1-0$ Transitions of the ^{13}C Isotopic Species of Cyanoacetylene (HCCCN) in the Direction of Sagittarius B2."
- M. Morris, W. Gilmore, P. Palmer, B. E. Turner, and B. Zuckerman, *Astrophys. J. (Letters)* **199**, L47 (1975). "Detection of Interstellar SiS and a Study of the IRC+ 10216 Molecular Envelope."
- P. T. Giguere and F. O. Clark, *Astrophys. J.* **198**, 761 (1975). "Radio Search for HC_3N , HCN, OH and Detection of U8.19 in Comet Kohoutek (1973f)."
- B. E. Turner, A. G. Kiszyakov, H. S. Liszt, and N. Kaifu, *Astrophys. J. (Letters)* **201**, L149 (1975). "Microwave Detection of Interstellar Cyanamide."
- R. S. McGee, L. M. Newton, and P. W. Butler, *Astrophys. J.* **202**, 76 (1975). "The 9.1 GHz Cyanoacetylene Line in Sagittarius B2."
- M. Morris, B. E. Turner, P. Palmer, and B. Zuckerman, *Astrophys. J.* **205**, 82 (1976). "Cyanoacetylene in Dense Interstellar Clouds."
- F. O. Clark, R. D. Brown, P. D. Godfrey, J. W. V. Storey, and D. R. Johnson, *Astrophys. J. (Letters)* **210**, L139 (1976). "Detection of Interstellar Vibrationally Excited Cyanoacetylene."
- E. Churchwell, C. M. Walmsley, and G. Winniewisser, *Astron. Astrophys.* **54**, 925 (1977). "Observational Evidence for Chemical Fractionation in Sgr B2: The ^{13}C -Isotopes of Cyanoacetylene."
- B. E. Turner, *Astrophys. J. (Letters)* **213**, L75 (1977). "Microwave Detection of Interstellar Ketene."