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Microwave Spectra of Molecules of Astrophysical Interest
X. Isocyanic Acid

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The available data on the microwave spectrum of isocyanic acid are critically reviewed for information applicable to radio astronomy. Molecular data such as rotational constants, centrifugal distortion parameters, dipole moments, hyperfine coupling constants, and structural parameters are tabulated. Detailed centrifugal distortion calculations have been carried out for all isotopic forms of this molecule, including DNCO. Transitions have been predicted for the parent molecule for the frequency range 160 MHz–300 GHz. All predicted transitions include error limits. The quoted uncertainties represent one standard deviation. A 95 percent confidence limit is obtained by using approximately twice the calculated standard deviation. Estimated error limits for the measured transitions are discussed. References are given for all data included.

Key words: Isocyanic acid; interstellar molecules; microwave spectra; molecular parameters; rotational transitions; radio astronomy.

Contents

1. Introduction

The present tables were prepared in response to the needs of the rapidly progressing field of molecular radio astronomy and are intended to update and revise the existing tabulated literature on molecules already identified in interstellar observations [1].[1] The spectral information reported includes predicted and observed transitions between 160 MHz and 300 GHz for five isotopic species of isocyanic acid: $H^{14}N^{12}C^{16}O$, $D^{14}N^{12}C^{16}O$, $H^{15}N^{12}C^{16}O$, $H^{14}N^{13}C^{16}O$ and $H^{14}N^{12}C^{18}O$. The frequency predictions for $H^{14}N^{12}C^{16}O$ and $D^{14}N^{12}C^{16}O$ are extensive and include transitions whose lower energy states are below 750 cm^{-1} and 250 cm^{-1}, respectively.[2] For the remaining isotopic species transitions of particular astrophysical interest are predicted. The deuterated species has been included in these tables, since it is conceivable that interstellar deutero-isocyanic acid may be observable.

[1] Figures in brackets indicate literature references in section 1.4.

[2] In keeping with the commonly accepted convention in molecular spectroscopy, the fundamental frequencies and vibrational energies are frequently expressed in their wavenumber (cm^{-1}) equivalents.

It is felt that these limits are generous enough to allow for the presentation of all transitions which might be observed by existing telescopes, or by those likely to be developed in the next several years.

1.1. Molecular Parameter Tables

The rotational constants and centrifugal distortion constants presented in tables 1, 2, and 3 were obtained from a least-squares analysis of the observed spectral lines with a computer program which includes centrifugal distortion terms, in addition to the basic rigid asymmetric rotor energy matrix. The very high rotational energies and large centrifugal distortion made it necessary to include high order terms (up to the twelfth power) in the angular momentum in the Hamiltonian. However, the small number of observable branches of isocyanic acid in the microwave and millimeter-wave regions meant that some low order distortion constants, in particular D_K and H_K, were indeterminate. The A_0 rotational constants given in tables 1–3 are thus effective constants which contain substantial contributions from the indeterminate distortion constants. All of the effective A_0 values were corrected for the largest distortion term (D_K-H_K) using the far infrared data [2] before calculation of the moments of inertia [3]. Details of the centrifugal distortion calculation and the statistical analysis used in this review have been discussed by Hocking, Gerry, and Winnewisser [3] as well as by Helminger, Cook, and de Lucia [4]. This formulation is similar to those discussed by Kirchoff [5] and by Steenbeckeliers [6]. As pointed out in earlier parts of this series, it is necessary to retain more significant figures in the spectral constants than indicated by the statistical error limits, if the constants are to reproduce the observed spectra to within experimental error.

1.2. Microwave Spectral Tables

Tables 4 through 9 contain the results of the statistical analysis of the rotational spectrum of $H^{14}N^{12}C^{16}O$, $D^{14}N^{12}C^{16}O$, $H^{14}N^{13}C^{16}O$, $H^{15}N^{12}C^{16}O$, and $H^{14}N^{12}C^{18}O$, respectively. For each spectral line in tables 4 and 5 the first column contains the upper state and lower state quantum number in the form JK_aK_c for a rigid asymmetric rotor plus the total angular momentum quantum number $F=J+I_1,\ J+I_1-1,\ .\ .\ .,\ J-I_1$, where I_1 is the nuclear spin angular momentum quantum number for the ^{14}N nucleus, with $I_1=1$. The quantum numbers are followed by the observed unsplit line frequency. The estimated experimental uncertainty is quoted in the footnote at the end of each table. The third column contains the calculated frequency and estimated uncertainty in MHz. The calculated uncertainties represent one standard deviation obtained from the least squares analysis. A 95 percent confidence limit on the predictions is obtained by using approximately twice (this varies slightly with the number of data included in the calculation) standard deviation of the calculated uncertainties. Underneath each rotational transition the F quantum numbers are given for all transitions whose total quadrupole splitting is larger than 50 kHz. Opposite the F quantum numbers the calculated splittings due to the nuclear electric quadrupole interaction are listed along with their estimated uncertainties in MHz. The calculated uncertainties represent one standard deviation. The actual transition frequencies can be obtained by adding the hyperfine splittings to the unsplit frequency, and the estimated error of each is then the root mean square of the individual estimated uncertainties.

Tables 7 and 8 contain essentially only the measured spectra of ^{13}C, ^{15}N, and ^{18}O labelled isocyanic acid together with the results of the statistical analysis and a selected number of predicted transitions. Further information is available from the authors on request. The line strengths for the unsplit rotational transitions are given in column 4. These line strengths, denoted by $^{x}S\ (J'_{K'_a,K'_c};\ J''_{K''_a,K''_c})$ are defined in this review as:

$$^{x}S\ (J'_{K'_a,K'_c};\ J''_{K''_a,K''_c})=\frac{(2J'+1)|\mu_{J'\leftarrow J''}|^2}{\mu_x^2},$$

where the superscript x refers to one of the principal axes of the molecule ($x=a$, b, or c); $|\mu_{J'\leftarrow J''}|$ is the dipole moment matrix element connecting the upper $J'_{K'_a,K'_c}$ and lower, $J''_{K''_a,K''_c}$, rotational levels involved in the transition, and μ_x is the magnitude of the component of μ along the x-axis. Thus, the line strength as defined is independent of the absolute magnitude of the dipole moment.

The total rotational energy of each rotational level was calculated using all distortion constants which were used in the analysis and quoted in tables 1, 2, and 3. These are given in columns 5 and 6 in cm^{-1}. The estimated accuracy of the calculated values for the energy levels are not better than: for $K_a=0$ about two decimal places, for $K_a=2$ about one decimal place, for $K_a=3$ about $\pm 1\ cm^{-1}$, $K_a=4$ about $\pm 3\ cm^{-1}$, and for $K_a=5$ about $\pm\ 7\ cm^{-1}$. No levels with $K\geqslant 6$ have been included, due to their general uncertainty, and they are also not likely to be observed astrophysically. Although the b-type transitions have been observed in the laboratory in the microwave and millimeter-wave regions, they are likely not to be detected astrophysically, due to their very high J quantum numbers. For completeness, they have, however, been included in the tables. If any further information is needed on these transitions, the authors of this review possess the necessary programs. The laboratory measurements are taken from ref. [75], unless quoted differently in the last column. As a convenience to the user, the calculated unsplit transition frequencies from table 4 for $H^{14}N^{12}C^{16}O$ have been listed according to increasing frequency in table 10. We have included in this table some low J high frequency b-type transitions. They may become of interest for the developing field of far infrared astronomy.

1.3. List of Symbols and Conversion Factors

a. Symbols

A, B, C	Rotational constants (MHz). $A \geq B \geq C$.
D, δ_J, R_6	Quartic centrifugal distortion constants.
H	Sextic centrifugal distortion constants.
L	Octic centrifugal distortion constants.
S	Dectic centrifugal distortion constants.
T	12th order centrifugal distortion constants.
a, b, c	Principal axes corresponding to A, B, C.
$\mu, \mu_x (x=a, b, c)$	Dipole moment and components of the dipole moment along the principal axes.
$eqQ_{aa}, \ldots$	Nuclear electric quadrupole coupling constant along indicated principal axis (MHz).
χ_{ij}	Elements of the quadrupole coupling tensor (MHz).
$r(X-Y)$	Distance between centers of mass of atom X and Y (Å).
$\measuredangle(X, Y, Z)$	Angle formed by atoms X, Y, and Z (degrees).
$I_{a,b,c}$	Moments of inertia of whole molecule with respect to the indicated principal axis.
F	Total angular momentum quantum number.
J	Total rotational angular momentum quantum number.
K_a	Projection of J on the symmetry axis in the limiting prolate symmetric top.
K_c	Projection of J on the symmetry axis in the limiting oblate symmetric top.
(. . .)	Parentheses in the numerical listings contain measured or estimated uncertainties. These should be interpreted as: $1.532(30)=1.532(0.030)=1.532\pm 0.030$.

b. Conversion Factors

The following conversion factors have been used:

$$A, B, C\ (\text{MHz}) = \frac{5.05375\times 10^5}{I_{a,b,c}(\text{amu Å}^2)}$$

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

c. Acknowledgements

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1.4. References

[1] D. R. Johnson, F. J. Lovas, and W. J. Kirchhoff, J. Phys. Chem. Ref. Data **1**, 1011 (1972).

[2] B. Krakow, R. C. Lord, and G. O. Neely, J. Mol. Spectrosc. **27**, 148 (1968).

[3] W. H. Hocking, M. C. L. Gerry, and G. Winnewisser, Can. J. Phys. (1975, in press).

[4] P. Helminger, R. L. Cook, and F. C. de Lucia, J. Chem. Phys. **56**, 4581 (1972).

[5] W. H. Kirchhoff, J. Mol. Spectrosc. **41**, 333 (1972).

[6] G. Steenbeckeliers, Ann. Soc. Sci. Brux. **82**, 331 (1968).

a. Primary Laboratory References

[51] J. N. Shoolery, R. G. Shulman, and D. M. Yost, J. Chem. Phy **19**, 250 (1951); "Dipole Moment and Electric Quadrupo. Effects in HNCO and HNCS."

[63] R. Kewley, K. V. L. N. Sastry, and M. Winnewisser, J. Mol. Spectrosc. **10**, 418 (1963). "The Millimeter Wave Spectra of Isocyanic and Isothiocyanic Acids."

[68] B. Krakow, R. C. Lord, and G. O. Neely, J. Mol. Spectrosc. **27**, 148 (1968). "A High Resolution Far Infrared Study of Rotation Spectra in HN_3, HNCO, and HNCS, and their Deuterium Derivatives."

[71] S. G. Kukolich, A. C. Nelson, and B. S. Yamanashi, J. Am. Chem. Soc. **93**, 6769 (1971). "Molecular-Beam Microwave Spectra of HNCO and DNCO."

[72A] W. H. Hocking, M. C. L. Gerry, and G. Winnewisser, Astrophys. J. **174**, L93 (1972). "Microwave Spectrum of Isocyanic Acid, HNCO."

[74] W. H. Hocking, M. C. L. Gerry, and G. Winnewisser, Astrophys. J. **187**, L89 (1974). "The Dipole Moment of Isocyanic Acid, HNCO, and its Astrophysical Consequences."

[75] W. H. Hocking, M. C. L. Gerry, and G. Winnewisser, preprint (1975), Can. J. Phys. (in press). "The Microwave and Millimeter-Wave Spectrum, Molecular Constants, Dipole Moment, and Structure of Isocyanic Acid, HNCO."

b. Other Laboratory References

[50A] G. Herzberg and C. Reid, Discussions Faraday Soc. **9**, 92 (1950). "Infrared Spectrum and Structure of the HNCO Molecule."

[50B] L. H. Jones, J. N. Shoolery, R. G. Shulman, and D. M. Yost, J. Chem. Phys. **18**, 990 (1950). "The Molecular Structure of Isocyanic Acid from Microwave and Infrared Absorption Spectra."

[65] C. R. Noller, Chemistry of Organic Compounds, 3rd ed. (Saunders, Philadelphia).

[67] K. J. White and R. L. Cook, J. Chem. Phys. **46**, 143 (1967). "Millimeter Wave Rotational Stark Spectra of HNCO, DNCO, and HN_3: Dipole Moment Changes with K."

[68] G. O. Neely, J. Mol. Spectrosc. **27**, 177 (1968). "Interpretation of Extreme Centrifugal Distortion in HNCO, HNCS, and Their Deuterium Derivatives."

[73A] W. H. Hocking, Ph. D. Thesis, The University of British Columbia, Vancouver, Canada (1973). "The Microwave Spectra and Structures of Some Isocyanates."

c. Interstellar References

[72B] L. E. Snyder and D. Buhl, New York, Acad. Sci. Annuals **194**, 17 (1972). "Detection of Several New Interstellar Molecules."

[72C] L. E. Snyder and D. Buhl, Astrophys. J. **177**, 619 (1972). "Interstellar Isocyanic Acid."

[72D] D. Buhl and L. E. Snyder, Mem. Soc. Roy. Liège **6**, 111, 481

(1972). "MM-Wave Lines of Organic Molecules."
[72E] D. Buhl, L. E. Snyder, and J. Edrich, Astrophys. J. **177**, 625 (1972). "An Interstellar Emission Line from HNCO at 1.4 cm."
[73B] L. E. Snyder and D. Buhl, Nature Phys. Sci. **243**, 45 (1973). "Interstellar Methylacetylene and Isocyanic Acid."
[73C] D. Buhl, L. E. Snyder, P. R. Schwartz, and J. Edrich, Nature **243**, 513 (1973). "HNCO in the Galactic Center."
[73D] P. M. Solomon, A. A. Penzias, K. B. Jefferts and R. W. Wilson, Astrophys. J. **185**, L63 (1973). "Millimeter Emission Lines of Polyatomic Molecules in Sagittarius B2."

2. Isocyanic Acid Spectral Tables

TABLE 1. Molecular Parameters for Isocyanic Acid

$H^{14}N^{12}C^{16}O$			
Rotational Constants[a] (MHz)			Ref. [75]
A_o	912 712.288 (136)		
B_o	11 071.01027 (62)		
C_o	10 910.57748 (64)		
Distortion Constants[a] (MHz)			Ref. [75]
D_J	-3.516609(3000)	$\times10^{-3}$	
D_{JK}	0.93376 (64)		
δ_J	7.30161 (890)	$\times10^{-5}$	
R_6	-2.264 (230)	$\times10^{-5}$	
H_J			
H_{JK}	1.569 (150)	$\times10^{-6}$	
H_{KJ}	3.32 (32)	$\times10^{-2}$	
L_{JK}			
L_{KJ}	-3.315 (49)	$\times10^{-3}$	
S_{KJ}	1.529 (29)	$\times10^{-4}$	
T_{KJ}	-2.650 (54)	$\times10^{-6}$	
D_K-H_K	4990 (400)		Ref. [68B]
Dipole Moment (Debye)			Ref. [75]
μ_a	1.575±0.005		
μ_b	1.35 ±0.10		

TABLE 1. Molecular Parameters for Isocyanic Acid —Continued

$H^{14}N^{12}C^{16}O$		
Nitrogen Quadrupole Coupling Constants (MHz)		
χ_{aa}	2.0527(10)	Ref. [71]
χ_{bb}	-0.473(7)	Ref. [75]
χ_{cc}	-1.583(7)	Ref. [75]
Moments of Inertia (amu Å^2)		
I_a^o =	0.55070	
I_b^o =	45.648499	
I_c^o =	46.319730	
Δ =	$I_c^o-I_b^o-I_a^o$ = 0.12053	
Structure		Ref. [75]
r(N-H) = 0.986 Å;		
r(N-C) = 1.209 Å;		
r(C-O) = 1.166 Å;		
∢(HNC) = 128.0°		
∢(NCO) = 180°		

[a] The numbers in parenthesis are standard errors in units of the last significant figures. See section 1.3A for interpretation of these standard deviations.

TABLE 2. Molecular Parameters for *Isocyanic Acid*

	$D^{14}N^{12}C^{16}O$	$H^{15}N^{12}C^{16}O$	
Rotational Constants[a] (MHz)			Ref. [75]
A_o	510 971.6806 (400)	902 803.34 (82.50)	
B_o	10 313.71371 (63)	10 737.8611(110)	
C_o	10 079.67647 (65)	10 585.4961(110)	
Distortion Constants[a] (MHz)			Ref. [75]
D_J	$3.29278(240)\times10^{-3}$	$4.149\ (260)\times10^{-3}$	
D_{JK}	-0.24510 (25)	1.0559 (93)	
δ_J	$2.04319(360)\times10^{-4}$	$6.2971(200)\times10^{-5}$	
R_6	$-3.66\ (23)\times10^{-5}$		
H_J	$-2.398\ (170)\times10^{-8}$	$2.74\ (59)\times10^{-6}$	
H_{JK}	$1.846\ (230)\times10^{-6}$	$8.73\ (1.90)\times10^{-4}$	
H_{KJ}	$-7.3431\ (430)\times10^{-3}$	$3.74\ (19)\times10^{-2}$	
L_{JK}		$-8.99\ (2.00)\times10^{-5}$	
L_{KJ}	$8.838\ (290)\times10^{-5}$	$-1.884\ (130)\times10^{-3}$	
S_{KJ}	$-9.60\ (77)\times10^{-7}$		
T_{KJ}	$4.70\ (70)\times10^{-9}$		
D_K-H_K	2700 (200)	4990 (400)	Ref. [68B]
Nitrogen Quadrupole Coupling Constants[a] (MHz)			
χ_{aa}	2.1230(10)		Ref. [71]
χ_{bb}	-0.540 (12)		Ref. [75]
χ_{cc}	-1.570 (12)		Ref. [75]
Deuterium Quadrupole Coupling Constant[a] *(kHz)*			
χ_{aa}	53.6 (2)		Ref. [71]

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

TABLE 3. Molecular Parameters for Isocyanic Acid

	$H^{14}N^{13}C^{16}O$	$H^{14}N^{12}C^{18}O$	
Rotational Constants[a] (MHz)			Ref. [75]
A_o	910 498.79 (1.21)	912 623.326 (400)	
B_o	11 071.48157(260)	10 470.8950 (12)	
C_o	10 910.73242(260)	10 327.2418 (12)	
Distortion Constants[a] (MHz)			Ref. [75]
D_J	$3.5387\ (93)\times10^{-3}$	$3.1588(55)\times10^{-3}$	
D_{JK}	0.9293 (31)	0.8196(11)	
δ_J	$7.320\ (30)\times10^{-5}$	$6.1215(93)\times10^{-5}$	
R_6	$-3.315(1000)\times10^{-5}$		
H_J			
H_{JK}		$-7.638(1.100)\times10^{-6}$	
H_{KJ}	$3.391\ (130)\times10^{-2}$	$2.653\ (51)\times10^{-2}$	
L_{JK}		$7.991(960)\times10^{-6}$	
L_{KJ}	$-3.409\ (190)\times10^{-3}$	$-2.252\ (67)\times10^{-3}$	
S_{KJ}	$1.55\ (11)\times10^{-4}$	$6.300(250)\times10^{-5}$	
T_{KJ}	$-2.64\ (20)\times10^{-6}$		
D_K-H_K	4990 (400)	4990(400)	Ref. [68B]
Nitrogen Quadrupole Coupling Constants (MHz)			Ref. [75]
χ_{aa}	2.067 (20)	2.060 (13)	
χ_{bb}	-0.402 (11)	-0.472 (8)	
χ_{cc}	-1.585 (11)	-1.588 (8)	

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

TABLE 4. The Microwave Spectrum of $H^{14}N^{12}C^{16}O$ (MHz)

(1) Transition J'	K'_a	K'_c	J"	K''_a	K''_c	(2) Observed (Est. Uncert.[c])	(3) Calculated + Quadrupole shifts (standard dev.)[d]	(4) Line strength + Rel. Intensity of Quadrupole comp.	Energy levels[a] in cm^{-1} upper state	lower state	(6) Ref.[b]
1	0	1	0	0	0		21981.574(1)	1.000	0.733	0.0	
	F'=	2		F"=	1	21981.47055	-0.103(1)	0.556			71
		1			1	21982.08535	0.514(3)	0.333			71
		0			1	21980.54533	-1.028(6)	0.111			71
2	0	2	1	0	1		43963.042(2)	2.000	2.200	0.733	
	F'=	3		F"=	2	43963.000	-0.044(0)	0.467			
		2			2	43963.626	0.617(3)	0.083			
		2			1	43963.000	0.000(0)	0.250			
		1			1	43962.007	-1.028(6)	0.083			
		1			0	43963.626	0.514(3)	0.111			
2	1	1	1	1	0		44119.879(2)	1.500	32.3	30.81	
	F'=	3		F"=	2	44119.757	-0.113(1)	0.467			
		2			2	44120.159	-0.039(2)	0.083			
		2			1	44120.390	0.514(3)	0.250			
		1			1	44119.903	-0.278(2)	0.083			
		1			0	44118.967	-0.910(4)	0.111			
2	1	2	1	1	1		43799.019(2)	1.500	32.3	30.81	
	F'=	3		F"=	2	43798.873	-0.137(1)	0.467			
		2			2	43799.423	0.372(2)	0.083			
		2			1	43799.533	0.514(3)	0.250			
		1			1		-0.278(2)	0.083			
		1			0	43798.360	-0.632(4)	0.111			
3	0	3	2	0	2	65944.301	65944.298(4)	3.000	4.399	2.200	
	F'=	4		F"=	3		-0.025(0)	0.429			
		3			2		0.000(0)	0.296			
		2			1		0.103(1)	0.200			
3	1	3	2	1	2		65698.308(3)	2.667	34.461	32.270	
	F'=	4		F"=	3	65698.262	-0.062(0)	0.429			
		2			1	65698.262	-0.024(0)	0.200			
		3			2	65698.439	0.129(1)	0.296			
3	1	2	2	1	1		66179.590(3)	2.667	34.49	32.29	
	F'=	4		F"=	3	66179.531	-0.049(0)	0.429			
		3			2	66179.729	0.129(1)	0.296			
		2			1	66179.531	-0.079(0)	0.200			
3	2	2	2	2	1		65924.118(3)	1.667	122.89	120.69	
	F'=	4		F"=	3	65294.015	-0.147(1)	0.429			

TABLE 4. Continued

(1)						(2)	(3)	(4)	(5)	(6)
		3			2	65924.679	0.514(3)	0.296		
		2			1	65923.626	-0.514(3)	0.200		
3	2	1	2	2	0		65924.199(3)	1.667	122.39	120.69
	F'=	4		F"=	3	65924.015	-0.147(1)	0.429		
		3			2	65924.679	0.514(3)	0.296		
		2			1	65923.626	-0.514(3)	0.200		
4	0	4	3	0	3	87925.252	87925.238(4)	4.000	7.332	4.399
	F'=	5		F"=	4		-0.016(0)	0.407		
		4			3		0.000(0)	0.313		
		3			2		0.044(0)	0.238		
4	1	4	3	1	3	87597.342	87597.333(3)	3.750	37.38	34.46
	F'=	5			4		-0.035(0)	0.407		
		4			3		0.051(0)	0.313		
		3			2		0.008(0)	0.238		
4	1	3	3	1	2	88239.036	88239.027(3)	3.750	37.44	34.49
	F'=	5		F"=	4		-0.026(0)	0.407		
		4			3		0.051(0)	0.313		
		3			2		-0.016(0)	0.238		
4	2	3	3	2	2		87898.416(4)	3.000	125.83	122.89
	F'=	5		F"=	4	87898.341	-0.075(0)	0.407		
		4			3	87898.565	0.206(1)	0.313		
		3			2	87898.341	-0.147(1)	0.238		
4	2	2	3	2	1		87898.620(4)	3.000	125.83	122.89
	F'=	5		F"=	4	87898.565	-0.075(0)	0.407		
		4			3	87898.840	0.206(1)	0.313		
		3			2	87898.565	-0.147(1)	0.238		
4	3	2	3	3	1		87867.280(5)	1.750	268.65	265.71
4	3	1	3	3	0		87867.280(5)	1.750	268.65	265.71
	F'=	5		F"=	4	87867.132	-0.149(1)	0.407		
		4			3	87867.732	0.463(3)	0.313		
		3			2	87866.892	-0.386(2)	0.238		
5	0	5	4	0	4	109905.758	109905.753(5)	5.000	10.998	7.332
5	1	5	4	1	4	109496.008	109496.007(4)	4.800	41.04	37.38
5	1	4	4	1	3	110298.080	110298.098(4)	4.800	41.12	37.43
5	2	4	4	2	3	109872.337	109872.366(5)	4.200	129.49	125.83
5	2	3	4	2	2	109872.765	109872.773(5)	4.200	129.49	125.82
	F'=	6		F"=	5		-0.044(0)	0.393		
		5			4		0.103(1)	0.320		
		4			3		-0.059(0)	0.259		

TABLE 4. Continued

(1)						(2)	(3)	(4)	(5)	(6)
5	3	3	4	3	2		109833.489(6)	3.200	272.31	268.65
5	3	2	4	3	1		109833.489(6)	3.200	272.31	268.65
	F'=	6		F"=	5	109833.391	-0.085(0)	0.394		
		5			4	109833.737	+0.231(1)	0.320		
		4			3	109833.391	-0.163(0)	0.259		
5	4	2	4	4	1		109778.700(7)	1.800	469.19	465.52
5	4	1	4	4	0		109778.700(7)	1.800	469.19	465.52
	F'=	6		F"=	5	109778.542	-0.143(1)	0.394		
		4			3		-0.308(2)	0.259		
		5			4	109779.129	0.411(2)	0.320		
6	0	6	5	0	5		131885.740(6)	6.000	15.398	10.998
6	1	6	5	1	5		131394.241(5)	5.833	45.42	41.04
6	1	5	5	1	4		132356.711(5)	5.833	45.53	41.12
6	2	5	5	2	4		131845.880(5)	5.333	133.89	129.49
6	2	4	5	2	3		131846.590(6)	5.333	133.89	129.49
	F'=	7		F"=	6		-0.028(0)	0.385		
		6			5		0.059(0)	0.324		
		5			4		-0.028(0)	0.273		
6	3	4	5	3	3		131799.292(7)	4.500	276.71	272.31
6	3	3	5	3	2		131799.292(7)	4.500	276.71	272.31
	F'=	7		F"=	6		-0.054(0)	0.385		
		6			5		0.132(1)	0.324		
		5			4		-0.083(0)	0.273		
6	4	3	5	4	2		131733.534(7)	3.333	473.58	469.19
6	4	2	5	4	1		131733.534(7)	3.333	473.58	469.19
	F'=	7		F"=	6		-0.089(0)	0.385		
		6			5		0.235(1)	0.324		
		5			4		-0.159(1)	0.273		
6	5	2	5	5	1		131640.747(9)	1.833	741.47	737.07
6	5	1	5	5	0		131640.747(9)	1.833	741.47	737.07
	F'=	7		F"=	6		-0.135(1)	0.385		
		6			5		0.367(2)	0.324		
		5			4		-0.257(1)	0.273		
7	0	7	6	0	6	153865.08	153865.092(6)	7.000	20.530	15.398
7	1	7	6	1	6	153291.84	153291.946(6)	6.857	50.53	45.42
7	1	6	6	1	5	154414.77	154414.776(6)	6.857	50.68	45.53
7	2	6	6	2	5	153818.87	153818.869(6)	6.429		
	F'=	8		F"=	7		-0.019(0)	0.378		
		7			6		0.037(0)	0.327		
		6			5		-0.015(0)	0.282		
7	2	5	6	2	4	153819.98	153820.007(7)	6.429	139.02	133.89
	F'=	8		F"=	7		-0.019(0)	0.378		
		7			6		0.037(0)	0.327		
		6			5		-0.015(0)	0.282		

TABLE 4. Continued

(1)						(2)	(3)	(4)	(5)	(6)
7	3	5	6	3	4	153764.59	153764.606(8)	5.714	281.84	276.71
7	3	4	6	3	3	153764.59	153764.606(8)	5.714	281.84	276.71
	F'=	8		F"=	7		-0.036(0)	0.378		
		7			6		0.083(0)	0.327		
		6			5		-0.047(0)	0.282		
7	4	4	6	4	3	153687.87	153687.873(7)	4.714	478.71	473.58
7	4	3	6	4	2	153687.87	153687.873(7)	4.714	478.71	473.58
	F'=	8		F"=	7		-0.060(0)	0.378		
		7			6		0.147(1)	0.327		
		6			5		-0.092(0)	0.282		
7	5	3	6	5	2	153579.62	153579.619(9)	3.429	746.59	741.46
7	5	2	6	5	1	153579.62	153579.619(9)	3.429	746.59	741.46
	F'=	8		F"=	7	153579.62	-0.090(0)	0.378		
		7			6		0.230(1)	0.327		
		6			5		-0.150(1)	0.282		
8	0	8	7	0	7	175843.701	175843.703(7)	8.000	26.395	20.530
8	1	8	7	1	7	175189.041	175189.037(8)	7.875	56.38	50.53
8	1	7	7	1	6	176472.204	176472.199(8)	7.875	56.57	50.68
8	2	7	7	2	6	175791.267	175791.248(7)	7.500	144.88	139.02
8	2	6	7	2	5	175792.957	175792.954(8)	7.500	144.88	139.02
8	3	6	7	3	5	175729.350	175729.350(9)	6.875	287.70	281.84
8	3	5	7	3	4	175729.350	175729.350(9)	6.875	287.70	281.84
	F'=	9		F"=	8		-0.026(0)	0.373		
		8			7		0.055(0)	0.328		
		7			6		-0.029(0)	0.289		
8	4	5	7	4	4	175641.671	175641.637(8)	6.000	484.6	478.7
8	4	4	7	4	3	175641.671	175641.637(8)	6.000	484.6	478.7
	F'=	9		F"=	8		-0.042(0)	0.373		
		8			7		0.098(1)	0.328		
		7			6		-0.058(0)	0.289		
8	5	4	7	5	3	175517.910	175517.913(8)	4.875	752.4	746.6
8	5	3	7	5	2	175517.910	175517.913(8)	4.875	752.4	746.6
	F'=	9		F"=	8		-0.063(0)	0.373		
		8			7		0.153(1)	0.328		
		7			6		-0.095(0)	0.289		
9	0	9	8	0	8	197821.39	197821.469(7)	9.000	32.994	26.395
9	1	9	8	1	8	197085.30	197085.424(10)	8.889	62.95	56.38
9	1	8	8	1	7	198529.03	198528.892(10)	8.889	63.19	56.57
9	2	8	8	2	7	197762.90	197762.928(9)	8.556	151.48	144.88
9	2	7	8	2	6	197765.30	197765.366(10)	8.556	151.48	144.88
9	3	7	8	3	6	197693.45	197693.444(10)	8.000	294.29	287.70
9	3	6	8	3	5	197693.45	197693.444(10)	8.000	294.29	287.70
9	4	6	8	4	5	197594.74	197594.741(9)	7.222	491.2	484.6
9	4	5	8	4	4	197594.74	197594.741(9)	7.222		

TABLE 4. Continued

(1)						(2)	(3)	(4)	(5)	(6)
10	0	10	9	0	9	219798.32	219798.282(8)	10.000	40.325	32.994
10	1	10	9	1	9	218981.17	218981.019(12)	9.900	70.25	62.95
10	1	9	9	1	8	220585.20	220584.762(12)	9.900	70.55	63.19
10	2	9	9	2	8	219733.850	219733.824(11)	9.600	158.81	151.48
10	2	8	9	2	7	219737.193	219737.175(13)	9.600	158.81	151.29
10	3	8	9	3	7	219656.71	219656.805(13)	9.100	301.62	294.29
10	3	7	9	3	6	219656.71	219656.805(13)	9.100	301.62	294.29
10	4	7	9	4	6	219547.082	219547.105(11)	8.400	498.5	491.2
10	4	6	9	4	5	219547.032	219547.105(11)	8.400	498.5	491.2
11	0	11	10	0	10		241774.037(10)	11.000	48.390	40.326
11	1	11	10	1	10		240875.735(16)	10.909	78.28	70.25
11	1	10	10	1	9		242639.717(16)	10.909	78.64	70.55
11	2	10	10	2	9		241703.846(15)	10.636	166.87	158.81
11	2	9	10	2	8		241708.315(17)	10.636	166.87	158.81
11	3	9	10	3	8		241619.351(16)	10.182	309.68	301.62
11	3	8	10	3	7		241619.353(16)	10.182	309.68	301.62
11	4	8	10	4	7		241498.644(15)	9.545	506.5	498.5
11	4	7	10	4	6		241498.644(15)	9.545	506.5	498.5
12	0	12	11	0	11		263748.630(13)	12.000	57.188	48.390
12	1	12	11	1	11		262769.484(20)	11.917	87.05	78.28
12	1	11	11	1	10		264693.665(20)	11.917	87.47	78.64
12	2	11	11	2	10		263672.909(20)	11.667	175.67	166.87
12	2	10	11	2	9		263678.717(22)	11.667	175.67	166.87
12	3	10	11	3	9		263581.003(21)	11.250	318.47	309.68
12	3	9	11	3	8		263581.006(21)	11.250	318.47	309.68
12	4	9	11	4	8		263449.276(20)	10.667	515.3	506.5
12	4	8	11	4	7		263449.276(20)	10.667	515.3	506.5
13	0	13	12	0	12		285721.952(17)	13.000	66.719	57.188
13	1	13	12	1	12		284662.177(25)	12.923	96.55	87.05
13	1	12	12	1	11		286746.515(25)	12.923	97.04	87.47
13	2	12	12	2	11		285640.924(26)	12.692	185.19	175.67
13	2	11	12	2	10		285648.316(29)	12.692	185.20	175.67
13	3	11	12	3	10		285541.677(27)	12.308	328.00	318.47
13	3	10	12	3	9		285541.681(27)	12.308	328.00	318.47
13	4	10	12	4	9		285398.921(27)	11.769	524.8	515.3
13	4	9	12	4	8		285398.921(27)	11.769	524.8	515.3
1	1	0	1	1	1		160.432(0)	1.500	30.814	30.809
	F'=	1		F"=	0		-0.632(4)	0.111		
		1			2		-0.419(2)	0.139		
		1			1		-0.278(2)	0.083		
		2			2		0.056(0)	0.417		
		2			1		0.197(2)	0.139		
		0			1		0.910(4)	0.111		
2	1	1	2	1	2		481.293(0)	0.833	32.286	32.270
	F'=	2		F"=	2		-0.278(2)	0.231		

TABLE 4. Continued

(1)						(2)	(3)	(4)	(5)	(6)
		3			3		0.079(1)	0.415		
		1			1		0.278(2)	0.150		
3	1	2	3	1	3		962.576(1)	0.583	34.493	34.461
	F'=	3		F"=	3		-0.278(3)	0.280		
		4			4		0.093(1)	0.402		
		2			2		0.222(2)	0.212		
4	1	3	4	1	4		1604.270(1)	0.450	37.437	37.383
	F'=	4		F"=	4		-0.278(2)	0.301		
		5			5		0.101(1)	0.391		
		3			3		0.198(1)	0.243		
5	1	4	5	1	5		2406.361(2)	0.367	41.116	41.035
	F'=	5		F"=	5		-0.278(2)	0.311		
		6			6		0.107(1)	0.383		
		4			4		0.185(1)	0.262		
6	1	5	6	1	6		3368.830(2)	0.310	45.531	45.418
	F'=	6		F"=	6		-0.278(2)	0.318		
		7			7		0.111(1)	0.377		
		5			5		0.177(1)	0.274		
7	1	6	7	1	7		4491.659(3)	0.268	50.681	50.532
	F'=	7		F"=	7		-0.276(2)	0.322		
		8			8		0.114(1)	0.372		
		6			6		0.171(1)	0.283		
8	1	7	8	1	8		5774.822(4)	0.236	56.568	56.375
	F'=	8		F"=	8		-0.278(2)	0.324		
		9			9		0.117(1)	0.368		
		7			7		0.167(1)	0.290		
9	1	8	9	1	9		7218.291(4)	0.211	63.190	62.949
	F'=	9		F"=	9		-0.278(2)	0.326		
		10			10		0.119(1)	0.365		
		8			8		0.163(1)	0.295		
10	1	9	10	1	10		8822.034(5)	0.191	70.548	70.254
	F'=	11		F"=	11	8822.20	0.121(1)	0.362		
		10			10	8821.78	-0.278(2)	0.327		
		9			9	8822.20	0.161(1)	0.299		
11	1	10	11	1	11		10586.015(5)	0.174	78.642	78.288
	F'=	12		F"=	12	10586.17	0.122(1)	0.360		
		11			11	10585.76	-0.278(2)	0.328		
		10			10	10586.17	0.159(1)	0.302		
12	1	11	12	1	12		12510.196(6)	0.160	87.471	87.053

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TABLE 4. Continued

(1)						(2)	(3)	(4)	(5)	(6)
	F'=	13		F"=	13	12510.35	0.123(1)	0.358		
		12			12	12509.92	-0.278(2)	0.329		
		11			11	12510.35	0.157(1)	0.305		
13	1	12	13	1	13		14594.535(6)	0.148	97.036	96.549
	F'=	14		F"=	14	14594.67	0.124(1)	0.356		
		13			13	14594.25	-0.278(2)	0.330		
		12			12	14594.67	0.155(1)	0.307		
14	1	13	14	1	14		16838.985(6)	0.138	107.336	106.774
	F'=	15		F"=	15	16839.12	0.125(1)	0.355		
		14			14	16838.71	-0.278(2)	0.330		
		13			13	16839.12	0.154(1)	0.309		
15	1	14	15	1	15		19243.496(6)	0.129	118.372	117.730
	F'=	16		F"=	16	19243.61	0.126(1)	0.353		
		15			15	19243.20	-0.278(2)	0.331		
		14			14	19243.61	0.153(1)	0.310		
16	1	15	16	1	16		21808.016(6)	0.121	130.143	129.416
	F'=	17		F"=	17	21808.16	0.127(1)	0.352		
		16			16	21807.75	-0.278(2)	0.331		
		15			15	21808.16	0.152(1)	0.312		
17	1	16	17	1	17		24532.487(6)	0.114	142.650	141.831
	F'=	18		F"=	18	24532.62	0.128(1)	0.351		
		17			17	24532.20	-0.278(2)	0.331		
		16			16	24532.62	0.151(1)	0.313		
18	1	17	18	1	18		27416.848(6)	0.108	155.892	154.978
	F'=	19		F"=	19	27417.00	0.128(1)	0.350		
		18			18	27416.58	-0.278(2)	0.331		
		17			17	27417.00	0.151(1)	0.314		
19	1	18	19	1	19		30461.036(7)	0.103	169.870	168.854
	F'=	20		F"=	20	30461.19	0.129(1)	0.350		
		19			19	30460.77	-0.278(2)	0.332		
		18			18	30461.19	0.150(1)	0.315		
20	1	19	20	1	20		33664.981(9)	0.098	184.583	183.460
	F'=	21		F"=	21	33665.12	0.129(1)	0.349		
		20			20	33664.70	-0.278(2)	0.332		
		19			19	33665.12	0.149(1)	0.316		
21	1	20	21	1	21		37028.612(12)	0.093	200.031	198.795
	F'=	22		F'=	22	37028.77	0.130(1)	0.348		
		21			21	37028.34	-0.278(2)	0.332		
		20			20	37028.77	0.149(1)	0.317		

TABLE 4. Continued

(1)						(2)	(3)	(4)	(5)	(6)
29	1	29	30	0	30	207631.364	207631.365(12)	14.819		
30	1	30	31	0	31	183318.380	183318.365(10)	15.352		
31	1	31	32	0	32		158934.883(8)	15.886		
32	1	32	33	0	33		134481.571(7)	16.423		
33	1	33	34	0	34	109959.087	109959.100(6)	16.961		
34	1	34	35	0	35	85369.134	85368.158(6)	17.502		
35	1	35	36	0	36		60709.448(6)	18.046		
	F' =	36		F" =	37	60709.339	-0.063(0)	0.342		
		35			36	60709.597	+0.131(1)	0.333		
		34			35	60709.399	-0.069(1)	0.324		
36	1	36	37	0	37	35983.71	35983.693(6)	18.592		
37	1	37	38	0	38	11191.64	11191.630(7)	19.140		
39	0	39	38	1	38	13666.02	13665.987(7)	19.691		
40	0	40	39	1	39		38588.382(7)	20.245		
41	0	41	40	1	40		63574.773(6)			
	F' =	42		F" =	41	63574.810	0.062(0)	0.342		
		41			40	63574.618	-0.130(1)	0.333		
		40			39	63574.810	0.068(1)	0.325		
42	0	42	41	1	41	88624.372	88624.352(6)			
43	0	43	42	1	42	113736.305	113736.298(7)			
44	0	44	43	1	43	138909.751	138909.772(8)			
45	0	45	44	1	44		164143.924(10)			
46	0	46	45	1	45	189437.889	189437.882(13)			
47	0	47	46	1	46	214790.736	214790.761(18)			

[a] The estimated accuracy of the height of the energy levels are as follows: for $K_a = 0$ about 2 decimal places; for $K_a = 1$, $K_a = 2$ about 1 decimal place; for $K_a = 3$ about ± 1 cm^{-1}; for $K_a = 4$ about ± 3 cm^{-1}; for $K_a = 5$ about ± 7 cm^{-1}.

[b] If there is no entry under References, then the data are taken from Ref. (75).

[c] The estimated experimental uncertainty in the measured transitions are: for the microwave transitions quoted to two decimal places ≤ ± 0.100 MHz, for millimeter wave transitions above 37 GHz quoted to two decimal places < ± 0.150 MHz, and for those quoted to three decimal places < ± 0.030 MHz.

[d] Note that one standard deviation is presented for the calculated uncertainty. These values should be multiplied by a factor of 2 to obtain ∿ 95% confidence level.

TABLE 5. The Microwave Spectrum of Isocyanic Acid-d. (MHz) ($D^{14}N^{12}C^{16}O$)

(1) Transition J'	K_a'	K_c'	J"	K_a''	K_c''	(2) Observed (Est. Uncert.[c])	(3) Calculated + Quadrupole shifts (standard dev.)[d]	(4) Line Strength + Rel. Intensity of Quadrupole comp.	(5) Energy levels[a] in cm^{-1} upper state	lower state	(6) Ref.[b]
1	0	1	0	0	0		20393.377(1)	1.000	0.680	0.0	
	F'=	2		F"=	1	20393.30	-0.106(1)	0.556			
		1			1	20393.91	0.528(4)	0.333			
		0			1	20392.40	-1.055(9)	0.111			
2	0	2	1	0	1		40786.593(2)	2.000	2.041	0.680	
	F'=	3		F"=	2	40786.568	-0.045(0)	0.467			
		2			2	40787.199	0.633(5)	0.083			
		2			1	40786.568	0.000(0)	0.250			
		1			1	40785.534	-1.055(9)	0.083			
		1			0	40787.199	0.527(4)	0.111			
2	1	1	1	1	0		41021.658(2)	1.500	18.757	17.388	
	F'=	3		F"=	2	41021.524	-0.117(1)	0.467			
		2			2	41021.918	0.056(3)	0.083			
		2			1	41022.186	0.528(4)	0.250			
		1			1	41021.704	0.258(4)	0.083			
		1			0	41020.699	-0.920(7)	0.111			
2	1	2	1	1	1		40553.596(2)	1.500	18.733	17.380	
	F'=	3		F"=	2	40553.456	-0.139(1)	0.467			
		2			2	40553.971	0.366(3)	0.083			
		2			1	40554.144	0.528(4)	0.250			
		1			1		-0.258(4)	0.083			
		1			0	40552.917	-0.662(7)	0.111			
3	0	3	2	0	2	61179.505	61179.488(3)	2.999	4.081	2.041	
3	1	3	2	1	2		60830.158(3)	2.667	20.762	18.733	
	F'=	4		F"=	3	60830.097	-0.063(0)	0.429			
		3			2	60830.291	0.132(1)	0.296			
		2			1	60830.097	-0.027(1)	0.200			
3	1	2	2	1	1		61532.226(3)	2.667	20.809	18.757	
	F'=	4		F"=	3	61532.156	-0.050(0)	0.429			
		3			2	61532.360	0.132(1)	0.296			
		2			1	61532.156	-0.079(1)	0.200			
3	2	2	2	2	1		61185.030(2)	1.667	69.91	67.87	
	F'=	4		F"=	3	61184.850	-0.151(1)	0.429			
		3			2	61185.547	0.528(4)	0.296			
		2			1	61184.479	-0.528(4)	0.200			
3	2	1	2	2	0		61185.351(2)	1.667	69.91	67.87	

TABLE 5. Continued

(1)						(2)	(3)	(4)	(5)		(6)
F'=		4	F"=		3	61185.188	0.151(1)	0.429			
		3			2	61185.869	0.527(4)	0.296			
		2			1	61184.850	-0.528(4)	0.200			
4	0	4	3	0	3	81571.913	81571.899(4)	3.998	6.802	4.081	
4	1	4	3	1	3	81106.420	81106.436(3)	3.750	23.468	20.762	
4	1	3	3	1	2	82042.469	82042.480(3)	2.750	23.546	20.809	
4	2	3	3	2	2		81579.612(2)	3.000	72.63	69.91	
F'=		5	F"=		4	81579.486	-0.077(1)	0.407			
		4			3	81579.812	0.211(2)	0.313			
		3			2	81579.486	-0.151(1)	0.238			
4	2	2	3	2	1		81580.415(3)	3.000	72.63	69.91	
F'=		5	F"=		4	81580.283	-0.077(1)	0.407			
		4			3	81580.614	0.211(2)	0.313			
		3			2	81580.283	-0.151(1)	0.238			
4	3	2	3	3	1		81586.243(4)	1.750	152.03	149.31	
4	3	1	3	3	0		81586.243(4)	1.750	152.03	149.31	
F'=		5	F"=		4	81586.072	-0.153(1)	0.407			
		4			3	81586.686	0.475(4)	0.313			
		3			2	81585.810	-0.396(3)	0.238			
5	0	5	4	0	4	101963.694	101963.666(5)	5.000	10.204	6.802	
5	1	5	4	1	4	101382.342	101382.335(4)	4.800	26.849	23.467	
5	1	4	4	1	3	102552.335	102552.317(4)	4.800	26.966	23.546	
5	2	4	4	2	3	101973.809	101973.828(3)	4.200	76.04	72.635	
5	2	3	4	2	2	101975.407	101975.433(3)	4.200	76.04	72.635	
5	3	2	4	3	1		101982.290(5)	3.200	155.43	152.03	
F'=		6	F"=		5	101982.155	-0.087(1)	0.394			
		5			4	101982.508	0.237(2)	0.320			
		4			3	101982.155	-0.167(1)	0.259			
5	4	2	4	4	1		101988.960(7)	1.800	264.61	261.21	
5	4	1	4	4	0		101988.960(7)	1.800	264.61	261.21	
F'=		6	F"=		5	101988.742	-0.147(1)	0.394			
		5			4	101989.369	0.422(3)	0.320			
		4			3		-0.317(3)	0.259			
6	0	6	5	0	5	122354.625	122354.626(5)	6.000	14.285	10.204	
6	1	6	5	1	5	121657.768	121657.761(4)	5.833	30.907	26.849	
6	1	5	5	1	4	123061.621	123061.631(4)	5.833	31.071	26.966	
6	2	5	5	2	4	122367.567	122367.584(4)	5.333	80.12	76.04	
6	2	4	5	2	3	122370.387	122370.393(4)	5.333	80.12	76.04	
6	3	4	5	3	3	122377.988	122377.995(5)	4.500	159.51	155.43	
6	3	3	5	3	2	122377.988	122377.995(5)	4.500	159.51	155.43	
F'=		7	F"=		6		-0.055(0)	0.385			
		6			5		0.136(1)	0.324			
		5			4		-0.085(1)	0.273			

TABLE 5. Continued

(1)						(2)	(3)	(4)	(5)	
6	4	3	5	4	2		122385.949(7)	3.333	268.69	264.61
6	4	2	5	4	1		122385.949(7)	3.333	268.69	264.61
	F' =	7		F" =	6	122385.856	-0.092(1)	0.385		
		6			5	122386.251	0.241(2)	0.324		
		5			4	122385.856	-0.163(1)	0.273		
7	0	7	6	0	6	142744.619	142744.622(6)	7.000	19.046	14.285
7	1	7	6	1	6	141932.599	141932.620(4)	6.857	35.642	30.907
7	1	6	6	1	5	143570.300	143570.318(4)	6.857	35.860	31.071
7	2	6	6	2	5	142760.781	142760.791(5)	6.429	84.88	80.118
7	2	5	6	2	4	142765.263	142765.285(5)	6.429	84.88	80.118
7	3	5	6	3	4	142773.280	142773.290(6)	5.714	164.27	159.51
7	3	4	6	3	3	142773.280	142773.292(6)	5.714	164.27	159.51
7	4	4	6	4	3	142782.475	142782.502(8)	4.714	273.45	268.69
7	4	3	6	4	2	142782.475	142782.502(8)	4.714	273.45	268.69
8	0	8	7	0	7	163133.522	163133.489(6)	8.000	24.488	19.046
8	1	8	7	1	7	162206.809	162206.817(4)	7.875	41.052	35.642
8	1	7	7	1	6	164078.251	164078.274(4)	7.875	41.333	35.860
8	2	7	7	2	6		163153.355(6)	7.500	90.32	84.88
8	2	6	7	2	5		163160.093(7)	7.500	90.32	84.88
8	3	6	7	3	5	163168.149	163168.103(7)	6.875	169.72	164.27
8	3	5	7	3	4	163168.149	163168.107(7)	6.875	169.72	164.27
8	4	5	7	4	4		163178.543(9)	6.000	278.90	273.45
8	4	4	7	4	3		163178.543(9)	6.000	278.90	273.45
9	0	9	8	0	8	183521.086	183521.069(6)	9.000	30.609	24.488
9	1	9	8	1	8	182480.240	182480.256(4)	8.889	47.139	41.052
9	1	8	8	1	7	184585.370	184585.392(4)	8.889	47.491	41.333
9	2	8	8	2	7	183545.171	183545.186(8)	8.559	96.44	90.32
9	2	7	8	2	6	183554.791	183554.809(9)	8.559	96.45	90.32
9	3	7	8	3	6	183562.372	183562.367(8)	8.000	175.84	169.72
9	3	6	8	3	5	183562.372	183562.374(8)	8.000	175.84	169.72
9	4	6	8	4	5	183574.022	183574.000(10)	7.222	285.02	278.90
9	4	5	8	4	4	183574.022	183574.000(10)	7.222	285.02	278.90
10	0	10	9	0	9	203907.209	203907.199(6)	10.000	37.411	30.609
10	1	10	9	1	9	202752.842	202752.843(5)	9.900	53.902	47.139
10	1	9	9	1	8	205091.551	205091.568(5)	9.900	54.331	47.491
10	2	9	9	2	8	203936.218	203936.189(11)	9.600	103.25	96.44
10	2	8	9	2	7		203949.419(12)	9.600	103.24	96.45
10	3	8	9	3	7	203956.028	203956.012(9)	9.100	182.64	175.84
10	3	7	9	3	6	203956.028	203956.025(9)	9.100	182.64	175.84
10	4	7	9	4	6		203968.799(11)	8.400	291.82	285.02
10	4	6	9	4	5		203968.799(11)	8.400	291.82	285.02
11	0	11	10	0	10	224291.760	224291.719(6)	11.000	44.893	37.411

TABLE 5. Continued

(1)						(2)	(3)	(4)	(5)	(6)
11	1	11	10	1	10		223024.484(6)	10.909	61.342	53.902
11	1	10	10	1	9		225596.697(6)	10.909	61.857	54.331
11	2	10	10	2	9	224326.267	224326.273(14)	10.636	110.73	103.25
11	2	9	10	2	8	224343.934	224343.909(16)	10.636	110.73	103.24
11	3	9	10	3	8	224349.026	224348.969(11)	10.182	190.13	182.64
11	3	8	10	3	7	224349.026	224348.990(11)	10.182	190.13	182.64
11	4	8	10	4	7	224362.883	224362.866(14)	9.545	299.31	291.82
11	4	7	10	4	6	224362.846	224362.866(16)	9.545	299.31	291.82
12	0	12	11	0	11	244674.487	244674.468(6)	12.000	53.054	44.892
12	1	12	11	1	11	243295.122	243295.083(8)	11.917	69.457	61.342
12	1	11	11	1	10	246100.655	246100.672(8)	11.917	70.066	61.857
12	2	11	11	2	10	244715.460	244715.346(18)	11.667	118.89	110.73
12	2	10	11	2	9	244738.382	244738.265(21)	11.667	118.90	110.73
12	3	10	11	3	9		244741.168(14)	11.250	198.29	190.13
12	3	9	11	3	8		244741.201(14)	11.250	198.29	190.13
12	4	9	11	4	8		244756.128(17)	10.667	307.47	299.31
12	4	8	11	4	7		244756.128(17)	10.667	307.47	299.31
13	0	13	12	0	12		265055.285(8)	13.000	61.895	53.054
13	1	13	12	1	12		263564.546(11)	12.923	78.249	69.457
13	1	12	12	1	11		266603.390(10)	12.923	78.959	70.066
13	2	12	12	2	11		265103.316(23)	12.692	127.74	118.89
13	3	11	12	3	10		265132.539(17)	12.308	207.13	198.29
13	3	10	12	3	9		265132.588(17)	12.308	207.13	198.29
13	4	10	12	4	9		265148.509(22)	11.769	316.32	307.47
13	4	9	12	4	8		265148.510(22)	11.769	316.32	307.47
13	2	11	12	2	10		265132.477(26)	12.692	127.74	118.90
1	1	0	1	1	1		234.035(0)	1.500	17.39	17.39
	F'=	1		F"=	0		-0.662(7)	0.111		
		1			2		-0.420(3)	0.139		
		1			1		-0.258(4)	0.083		
		2			2		0.052(1)	0.417		
		2			1		0.213(4)	0.139		
		0			1		0.920(7)	0.111		
2	1	1	2	1	2		702.097(1)	0.833	18.76	18.73
	F'=	2		F"=	2		-0.258(4)	0.231		
		3			3		0.074(1)	0.415		
		1			1		0.258(4)	0.150		
3	1	2	3	1	3		1404.165(2)	0.583	20.81	20.76
	F'=	3		F"=	3		-0.258(4)	0.280		
		4			4		0.086(1)	0.402		
		2			2		0.206(4)	0.212		
4	1	3	4	1	4		2340.208(3)	0.450	23.55	23.47
	F'=	4		F"=	4		-0.258(4)	0.301		
		5			5		0.094(2)	0.39		

TABLE 5. Continued

(1)						(2)	(3)	(4)	(5)		(6)
		3			3		0.184(3)	0.243			
5	1	4	5	1	5		3510.190(4)	0.367	26.97	26.85	
	F'=	5		F"=	5		-0.258(4)	0.311			
		6			6		0.099(2)	0.383			
		4			4		0.172(3)	0.267			
6	1	5	6	1	6		4914.060(5)	0.310	31.07	30.91	
	F'=	6		F"=	6		-0.258(4)	0.318			
		7			7		0.103(2)	0.377			
		5			5		0.164(3)	0.274			
7	1	6	7	1	7		6551.758(7)	0.268	35.86	35.64	
	F'=	7		F"=	7		-0.258(4)	0.322			
		8			8		0.106(2)	0.372			
		6			6		0.159(3)	0.283			
8	1	7	8	1	8		8423.215(8)	0.236	41.333	41.052	
	F'=	9		F"=	9	8423.34	0.109(2)	0.368			
		8			8	8422.96	-0.258(4)	0.324			
		7			7	8423.34	0.154(3)	0.290			
9	1	8	9	1	9		10528.351(9)	0.211	47.491	47.139	
	F'=	10		F"=	10	10528.48	0.111(2)	0.365			
		9			9	10528.11	-0.258(4)	0.326			
		8			8	10528.48	0.152(3)	0.295			
10	1	9	10	1	10		12867.076(9)	0.191	54.332	53.902	
	F'=	11		F"=	11	12867.19	0.112(2)	0.362			
		10			10	12866.80	-0.258(4)	0.327			
		9			9	12867.19	0.149(3)	0.299			
11	1	10	11	1	11		15439.289(9)	0.174	61.857	61.342	
	F'=	12		F"=	12	15439.41	0.113(2)	0.360			
		11			11	15439.03	-0.258(4)	0.328			
		10			10	15439.41	0.147(3)	0.302			
12	1	11	12	1	12		18244.878(9)	0.160	70.066	69.457	
	F'=	13		F"=	13	18245.02	0.115(2)	0.358			
		12			12	18244.60	-0.258(4)	0.329			
		11			11	18245.02	0.146(2)	0.305			
13	1	12	13	1	13		21283.722(8)	0.143	78.959	78.249	
	F'=	14		F"=	14	21283.85	0.116(2)	0.355			
		13			13	21283.47	-0.258(4)	0.330			
		12			12	21283.85	0.144(2)	0.307			
14	1	13	14	1	14		24555.687(9)	0.133	88.535	87.716	
	F'=	15		F"=	15	24555.85	0.116(2)	0.355			

TABLE 5. Continued

(1)						(2)	(3)	(4)	(5)	(6)
		14			14	24555.42	-0.258(4)	0.330		
		13			13	24555.85	0.143(2)	0.309		
15	1	14	15	1	15		28060.627(11)	0.129	98.796	97.860
	F'=	16		F"=	16	28060.77	0.117(2)	0.353		
		15			15	28060.39	-0.258(4)	0.331		
		14			14	28060.77	0.142(2)	0.310		
16	1	15	16	1	16		31798.387(17)	0.121	109.740	108.680
	F'=	17		F"=	17	31798.52	0.118(2)	0.352		
		16			16	31798.15	-0.258(4)	0.331		
		15			15	31798.52	0.141(2)	0.312		
13	1	13	14	0	14	204827.236	204827.248(14)	6.591		
14	1	14	15	0	15	182849.512	182849.547(12)	7.112		
15	1	15	16	0	16		160764.694(11)	7.635		
16	1	16	17	0	17	138573.857	138573.843(10)	8.160		
17	1	17	18	0	18	116278.174	116278.212(9)	8.689		
18	1	18	19	0	19	93879.120	93879.084(10)	9.221		
19	1	19	20	0	20		71377.807(10)	9.757		
20	1	20	21	0	21		48775.793(11)	10.296		
21	1	21	22	0	22	26074.49	26074.517(12)	10.839		
22	1	22	23	0	23		3275.520(14)	11.386		
24	0	24	23	1	23	19619.58	19619.597(15)	11.937		
25	0	25	24	1	24		42609.168(16)	12.493		
26	0	26	25	1	25		65691.469(17)	13.053		
27	0	27	26	1	26	88864.56	88864.708(17)	13.617		
28	0	28	27	1	27		112127.039(16)	14.186		
29	0	29	28	1	28		135476.553(15)	14.760		
30	0	30	29	1	29		158911.284(14)	15.339		
31	0	31	30	1	30	182429.187	182429.206(14)	15.924		
32	0	32	31	1	31	206028.254	206028.237(17)	16.514		
33	0	33	32	1	32		229706.240(25)	17.109		

[a] The estimated accuracy of the height of the energy levels are as follows: for K_a = 0 about 2 decimal places; for K_a = 1, K_a = 2 about 1 decimal place; for K_a = 3 about ± 1 cm^{-1}; for K_a = 4 about ± 3 cm^{-1}; for K_a = 5 about ± 7 cm^{-1}.

[b] If there is no entry under References, then the data are taken from Ref. (75).

[c] The estimated experimental uncertainty in the measured transitions are: for the microwave transitions quoted to two decimal places ≤ ± 0.100 MHz, for millimeter wave transitions above 37 GHz quoted to two decimal places < ± 0.150 MHz, and for those quoted to three decimal places < ± 0.030 MHz.

[d] Note that one standard deviation is presented for the calculated uncertainty. These values should be multiplied by a factor of 2 to obtain ∿ 95% confidence level.

TABLE 6. Molecular Beam Measurements on $D^{14}N^{12}C^{16}O$

Transition	F'_N	F'_D	Frequency (kHz)	Ref.
$1_{01} - 0_{00}$	0		20 392314.60(50)	71
	2	3	20 393270.18(50)	71
	2	2	20 393281.93(50)	71
	1	1	20 393901.83(50)	71
	1	2	20 393909.20(50)	71
	1	0	20 393921.63(50)	71
eqQ_{D-N} = 345(2) kHz				71
$eqQ(1_{01})$ = 2123.0 (1.0) kHz				71

TABLE 7. The Microwave Spectrum of Isocyanic Acid $H^{14}N^{13}C^{16}O$ (MHz)[c]

(1) Transition J'	K'_a	K'_c	J"	K''_a	K''_c	(2) Observed (Est. Uncert.[a])	(3) Calculated + Quadrupole shifts (Standard dev.)[b]
1	0	1	0	0	0		21982.200(5)
	F'=	2		F"=	1	21982.00	-0.103(1)
		1			1	21982.70	0.517(5)
		0			1	21981.15	-1.034(10)
2	0	2	1	0	1		43964.293(10)
2	1	2	1	1	1		43799.974(5)
2	1	1	1	1	0		44121.467(5)
3	0	3	2	0	2		65946.174(15)
3	1	3	2	1	2		65699.739(7)
3	1	2	2	1	1		66181.971(7)
3	2	2	2	2	1		65926.127(10)
3	2	1	2	2	0		65926.207(10)
4	0	4	3	0	3	87927.64	87927.736(19)
4	1	4	3	1	3	87599.12	87599.239(9)
4	1	3	3	1	2	88242.23	88242.199(9)
4	2	3	3	2	2		87901.094(13)
4	2	2	3	2	1		87901.293(13)
4	3	2	3	3	1		87870.058(17)
4	3	1	3	3	0		87870.058(17)
5	0	5	4	0	4	109908.95	109908.871(22)
5	1	5	4	1	4	109498.34	109498.384(11)
5	1	4	4	1	3	110301.98	110302.057(11)
5	2	4	4	2	3	109875.73	109875.709(16)
5	2	3	4	2	2	109876.08	109876.108(15)
5	3		4	3		109837.02	109836.955(20)
6	0	6	5	0	5		131889.474(24)
6	1	6	5	1	5		131397.087(13)
6	1	5	5	1	4		132361.456(13)
7	0	7	6	0	6	153869.52	152869.438(25)
7	1	7	6	1	6	153295.22	153295.259(16)
7	1	6	6	1	5	154420.46	154420.301(16)
7	2	6	6	2	5	153823.56	153823.536(24)
7	2	5	6	2	4	153824.66	153824.654(23)
7	3		6	3		153769.39	153769.435(27)
8	0	8	7	0	7	175848.57	175848.657(26)
8	1	8	7	1	7	175192.81	175192.811(21)
8	1	7	7	1	6	176478.51	176478.503(21)
8	2	6	7	2	5	175798.20	175790.249(30)
8	3		7	3		175734.83	175734.852(30)
8	4		7	4		175646.34	175646.340(56)
8	2	7	7	2	6	175796.53	175796.573(30)
9	0	9	8	0	8	197827.07	197827.025(26)
9	1	9	8	1	8	197089.60	197089.653(27)
9	1	8	8	1	7	198536.00	198535.969(27)
9	2	8	8	2	7	197760.93	197760.900(30)
9	2	7	8	2	6	197771.34	197771.301(39)
9	3		8	3		197699.63	197699.611(34)
9	4		8	4			197600.003(63)
9	5		8	5		197459.20	197459.200(56)
10	0	10	9	0	9		219804.434(25)
10	1	10	9	1	9		218985.700(35)
10	1	9	9	1	8		220592.604(35)
11	0	11	10	0	10		241780.779(26)
11	1	11	10	1	10		240880.861(45)
11	1	10	10	1	9		242648.320(45)
1	1	0	1	1	1		160.749(0)
	F'=	1		F"=	0		-0.637(8)
		1			2		-0.420(3)
		1			1		-0.276(3)
		2			2		0.055(1)
		2			1		0.200(3)
		0			1		0.913(8)
2	1	1	2	1	2		482.242(1)
	F'=	2		F"=	2		-0.276(3)
		3			3		0.079(1)
		1			1		0.276(3)
3	1	2	3	1	3		964.474(2)
	F'=	3		F"=	3		-0.276(3)
		4			4		0.092(1)
		2			2		0.221(2)
4	1	3	4	1	4		1607.433(4)
	F'=	4		F"=	4		-0.276(3)
		5			5		0.100(1)
		3			3		0.197(2)
5	1	4	5	1	5		2411.106(6)
	F'=	5		F"=	5		-0.276(3)

TABLE 7. Continued

(1) J'	K'_a	K'_c	J"	K''_a	K''_c	(2)	(3)
		6			6		0.106(1)
		4			4		0.184(2)
6	1	5	6	1	6		3375.474(8)
	F'=	6		F"=	6		-0.276(3)
		7			7		0.110(1)
		5			5		0.176(2)
7	1	6	7	1	7		4500.517(10)
	F'=	7		F"=	7		-0.276(3)
		8			8		0.114(1)
		6			6		0.170(2)
8	1	7	8	1	8		5786.210(12)
	F'=	8		F"=	8		-0.276(3)
		9			9		0.116(1)
		7			7		0.165(2)
9	1	8	9	1	9		7232.525(14)
	F'=	9		F"=	9		-0.276(3)
		10			10		0.118(1)
		8			8		0.162(2)
10	1	9	10	1	10		8839.430(16)
	F'=	11		F"=	11	8839.57	0.120(1)
		10			10	8839.16	-0.276(3)
		9			9	8839.57	0.160(1)
11	1	10	11	1	11		10606.890(18)
	F'=	12		F"=	12	10607.04	0.121(1)
		11			11	10606.63	-0.276(3)
		10			10	10607.04	0.158(1)
12	1	11	12	1	12		12534.865(19)
	F'=	13		F"=	13	12535.01	0.123(1)
		12			12	12534.60	-0.276(3)
		11			11	12535.01	0.156(1)
13	1	12	13	1	13		14623.314(20)
	F'=	14		F"=	14	14623.46	0.124(1)
		13			13	14623.04	-0.276(3)
		12			12	14623.46	0.154(1)
14	1	13	14	1	14		16872.189(20)
	F'=	15		F"=	15	16872.34	0.125(1)
		14			14	16871.92	-0.276(3)
		13			13	16872.34	0.153(1)
15	1	14	15	1	15		19281.441(20)
	F'=	16		F"=	16	19281.57	0.125(1)
		15			15	19281.16	-0.276(3)
		14			14	19281.57	0.152(1)
16	1	15	16	1	16		21851.019(20)
	F'=	17		F"=	17	21851.16	0.126(1)
		16			16	21850.77	-0.276(3)
		15			15	21851.16	0.151(1)
17	1	16	17	1	17		24580.863(19)
	F'=	18		F"=	18	24580.97	0.127(1)
		17			17	24580.52	-0.276(3)
		16			16	24580.97	0.150(1)
18	1	17	18	1	18		27470.912(19)
	F'=	19		F"=	19	27471.05	0.127(1)
		18			18	27470.64	-0.276(3)
		17			17	27471.05	0.150(1)
19	1	18	19	1	19		30521.103(22)
	F'=	20		F"=	20	30521.25	0.128(1)
		19			19	30520.83	-0.276(3)
		18			18	30521.25	0.149(1)
20	1	19	20	1	20		33731.369(29)
	F'=	21		F"=	21	33731.53	0.128(1)
		20			20	33731.11	-0.276(3)
		19			19	33731.53	0.149(1)
21	1	20	21	1	21		37101.635(39)
	F'=	22		F"=	22	37101.79	0.129(1)
		21			21	37101.38	-0.276(3)
		20			20	37101.79	0.148(1)
36	1	36	37	0	37	33658.44	33658.455(50)
37	1	37	38	0	38	8861.31	8861.288(32)
39	0	39	38	1	38	16001.52	16001.513(51)

[a] The estimated experimental uncertainty in the measured transitions are: for the microwave transitions quoted to two decimal places ≤ ± 0.100 MHz, for millimeter wave transitions above 37 GHz quoted to two decimal places < ± 0.150 MHz.

[b] Note that one standard deviation is presented for the calculated uncertainty. These values should be multiplied by a factor of 2 to obtain ∿ 95 % confidence level.

[c] The calculated hyperfine quadrupole shifts of all transitions of $HN^{13}C^{16}O$ agree to within ≤ 6 kHz with those calculated for $H^{14}N^{12}C^{16}O$ quoted in Table 4. Since this difference lies well within the accuracy of astronomical observations, quadrupole shifts are reproduced for certain transitions only, where splittings have been observed in the laboratory. Otherwise the reader is referred to Table 4.

TABLE 8. The Microwave Spectrum of Isocyanic Acid $H^{15}N^{12}C^{16}O$ (MHz)

Transition J'	K'_a	K'_c	J''	K''_a	K''_c	Observed (Est. Uncert.[a])	Calculated + Quadrupole shifts (Standard Dev.)[b]
1	0	1	0	0	0	21323.35	21323.341(20)
2	0	2	1	0	1		42646.563(35)
2	1	2	1	1	1		42490.163(25)
2	1	1	1	1	0		42794.889(25)
3	0	3	2	0	2		63969.549(38)
3	1	3	2	1	2		63735.038(28)
3	1	2	2	1	1		64192.119(28)
3	2	2	2	2	1		63947.377(49)
3	2	1	2	2	0		63947.455(49)
4	0	4	3	0	3	85292.129	85292.189(30)
4	1	4	3	1	3	84979.725	84979.670(23)
4	1	3	3	1	2	85589.122	85589.097(23)
4	2	3	3	2	2	85263.095	85262.932(37)
4	2	2	3	2	1	85263.095	85263.127(37)
4	3		3	3		85229.812	85229.807(39)
5	0	5	4	0	4	106614.42	106614.374(35)
5	1	5	4	1	4	106223.92	106223.986(24)
5	1	4	4	1	3	106985.75	106985.748(24)
5	2	4	4	2	3	106578.32	106578.294(37)
5	2	3	4	2	2		106578.684(37)
5	3		4	3		106536.66	106536.664(39)
5	4		4	4			106459.960(1826)
1	1	0	1	1	1		152.365(0)
2	1	1	2	1	2		457.090(1)
3	1	2	3	1	3		914.172(2)
4	1	3	4	1	4		1523.599(3)
5	1	4	5	1	5		2285.361(4)
6	1	5	6	1	6		3199.443(5)
7	1	6	7	1	7		4265.824(7)
8	1	7	8	1	8		5484.485(9)
9	1	8	9	1	9		6855.403(10)
10	1	9	10	1	10	8378.53	8378.547(11)
11	1	10	11	1	11	10053.88	10053.889(13)
12	1	11	12	1	12	11881.40	11881.396(14)
13	1	12	13	1	13	13861.02	13861.028(14)
14	1	13	14	1	14	15992.74	15992.749(14)
15	1	14	15	1	15	18276.54	18276.514(14)
16	1	15	16	1	16	20712.25	20712.276(14)
17	1	16	17	1	17	23300.01	23299.988(13)
18	1	17	18	1	18	26039.61	26039.595(13)
19	1	18	19	1	19	28931.02	28031.042(15)
20	1	19	20	1	20	31974.31	31974.271(20)
21	1	20	21	1	21	35169.19	35169.218(27)
37	1	37	38	0	38	29522.18	29522.181(39)
38	1	38	39	0	39		5452.468(55)
40	0	40	39	1	39	18684.61	18684.609(39)

[a] The estimated experimental uncertainty in the measured transitions are: for the microwave transitions quoted to two decimal places ≤ ± 0.100 MHz, for millimeter wave transitions above 37 GHz quoted to two decimal places < ± 0.150 MHz, and for those quoted to three decimal places < ± 0.030 MHz.

[b] Note that one standard deviation is presented for the calculated uncertainty. These values should be multiplied by a factor of 2 to obtain ∿ 95% confidence level.

TABLE 9. The Microwave Spectrum of Isocyanic Acid $H^{14}N^{12}C^{18}O$ (MHz)

(1) Transition J'	K'_a	K'_c	J''	K''_a	K''_c	(2) Observed Est. Uncert.[a]	(3) Calculated + Quadrupole shifts (Standard dev.)[b]
1	0	1	0	0	0		20798.124(2)
	F'=	2		F"=	1	20798.03	-0.103(1)
		1			1	20798.64	0.515(3)
		0			1	20797.11	-1.030(6)
2	0	2	1	0	1		41596.156(5)
	F'=	3		F"=	2	41596.132	-0.044(0)
		2			2	41596.725	0.618(4)
		2			1	41596.132	0.000(0)
		1			1	41595.142	-1.030(6)
		1			0	41596.725	0.515(3)
2	1	2	1	1	1		41449.341(3)
	F'=	3		F"=	2	41449.198	-0.137(1)
		2			2		0.374(2)
		2			1	41449.840	0.515(3)
		1			1		-0.279(3)
		1			0	41448.666	-0.633(5)
2	1	1	1	1	0		41736.643(3)
	F'=	3		F"=	2	41736.575	-0.113(1)
		2			2		0.038(2)
		2			1	41737.193	0.515(3)
		1			1		0.279(3)
		1			0	41735.763	-0.912(5)
3	0	3	2	0	2	62393.997	62394.001(7)
	F'=	4		F"=	3		-0.025(0)
		3			2		0.000(0)
		2			1		0.103(1)
3	1	3	2	1	2		62173.814(4)
	F'=	4		F"=	3	62173.751	-0.062(0)
		3			2	62173.927	0.129(1)
		2			1	62173.751	-0.024(0)
3	1	2	2	1	1		62604.761(4)
	F'=	4		F"=	3	62604.693	-0.049(0)
		3			2	62604.872	0.129(1)
		2			1	62604.693	-0.079(0)
3	2	2	2	2	1		62376.189(10)
	F'=	4		F"=	3	62376.095	-0.147(1)
		3			2	62376.750	0.515(3)
		2			1	62375.710	-0.515(3)
3	2	1	2	2	0		62376.257(10)
	F"=	4		F"=	3	62376.095	-0.147(1)
		3			2	62376.750	0.515(3)
		2			1	62375.710	-0.515(3)
4	0	4	3	0	3	83191.568	83191.567(9)
4	1	4	3	1	3	82898.038	82898.052(5)
4	1	3	3	1	2	83472.641	83472.633(5)
4	2	3	3	2	2		83167.895(12)
4	2	2	3	2	1		83168.067(12)
4	3	2	3	3	1		83140.275(14)
4	3	1	3	3	0		83140.275(14)
	F'=	5		F"=	4	83140.181	-0.149(1)
		4			3	83140.765	0.464(3)
		3			2	83139.922	-0.386(2)
5	0	5	4	0	4	103988.774	103988.761(10)
5	1	5	4	1	4	103621.974	103621.975(7)
5	1	4	4	1	3	104340.185	104340.179(7)
5	2	4	4	2	3	103959.293	103959.290(14)
5	2	3	4	2	2	103959.620	103959.639(14)
5	3	3	4	3	2		103924.895(16)
5	3	2	4	3	1		103924.895(16)
	F'=	6		F"=	5	103924.751	-0.085(1)
		5			4	103925.087	0.333(1)
		4			3	103924.751	-0.163(1)
5	4		4	4			103875.938(20)
	F'=	6		F"=	5	103875.730	-0.143(1)
		5			4	103876.331	0.412(3)
		4			3	103875.730	-0.309(2)
10	0	10	9	0	9	207966.18	207965.903(14)
10	1	10	9	1	9	207233.95	207234.123(19)
10	1	9	9	1	8	208670.16	208670.164(19)
10	2	9	9	2	8	207909.04	207909.050(14)
10	2	8	9	2	7	207911.90	207911.879(14)

TABLE 9 – Continued

(1)		(2)	(3)
1 1 0	1 1 1		143.653(0)
F'= 1	F"= 0		-0.633(5)
1	2		-0.421(2)
1	1		-0.279(3)
2	2		0.056(1)
2	1		0.197(2)
0	1		0.912(5)
2 1 1	2 1 2		430.956(0)
F'= 2	F"= 2		-0.279(3)
3	3		0.080(1)
1	1		0.279(3)
3 1 2	3 1 3		861.901(1)
F'= 3	F"= 3		-0.279(1)
4	4		0.093(1)
2	2		0.223(2)
4 1 3	4 1 4		1436.482(1)
F'= 4	F"= 4		-0.279(3)
5	5		0.102(1)
3	3		0.200(2)
5 1 4	5 1 5		2154.688(2)
F'= 5	F"= 5		-0.279(3)
6	6		0.107(1)
4	4		0.186(2)
6 1 5	6 1 6		3016.501(3)
F'= 6	F"= 6		-0.279(3)
7	7		0.112(1)
5	5		0.178(2)
7 1 6	7 1 7		4021.905(4)
F'= 7	F"= 7		-0.279(3)
8	8		0.115(1)
6	6		0.172(2)
8 1 7	8 1 8		5170.879(5)
F'= 8	F"= 8		-0.279(3)
9	9		0.118(1)
7	7		0.168(2)
9 1 8	9 1 9		6463.400(5)
F'= 9	F"= 9		-0.279(3)
10	10		0.120(1)
8	8		0.164(2)
10 1 9	10 1 10		7899.442(6)
F'=10	F"=10		-0.279(3)
11	11		0.121(1)
9	9		0.162(2)
11 1 10	11 1 11		9478.974(7)
F'=12	F"=12	9479.12	0.123(1)
11	11	9478.71	-0.279(3)
10	10	9479.12	0.160(2)
12 1 11	12 1 12		11201.963(8)
F"=13	F"=13	11202.11	0.124(1)
12	12	11201.69	-0.279(3)
11	11	11202.11	0.158(2)
13 1 12	13 1 13		13068.375(8)
F'=14	F"=14		0.125(1)
13	13		-0.279(3)
12	12		0.156(2)
14 1 13	14 1 14		15078.170(8)
F'=15	F"=15	15078.32	0.126(1)
14	14	15077.91	-0.279(3)
13	13	15078.32	0.155(2)
15 1 14	15 1 15		17231.307(8)
F'=16	F"=16	17231.45	0.127(1)
15	15	17231.04	-0.279(3)
14	14	17321.45	0.154(2)
16 1 15	16 1 16		19527.742(8)
F'=17	F"=17	19527.87	0.128(1)
16	16	19527.43	-0.279(3)
15	15	19527.87	0.153(2)
17 1 16	17 1 17		21967.425(8)
F'=18	F"=18	21967.58	0.128(1)
17	17	21967.15	-0.279(3)
16	16	21967.58	0.152(2)
18 1 17	18 1 18		24550.307(7)
F'=19	F"=19		0.129(1)
18	18		-0.279(3)
17	17		0.152(2)
19 1 18	19 1 19		27276.333(7)
F'=20	F"=20	27276.46	0.129(1)
19	19	27276.03	-0.279(3)
18	18	27276.46	0.151(2)
20 1 19	20 1 20		30145.445(8)
F'=21	F"=21	30145.62	0.130(1)
20	20	30145.18	-0.279(3)
19	19	30145.62	0.150(2)
21 1 20	21 1 21		33157.584(11)
F'=22	F"=22	33157.74	0.130(1)
21	21	33157.32	-0.279(3)
20	20	33157.74	0.150(2)
22 1 21	22 1 22		36312.684(14)
F'=23	F"=23	36312.81	0.131(1)
22	22	36312.41	-0.279(3)
21	21	36312.81	0.149(2)

TABLE 9 – Continued

(1)		(2)	(3)
35 1 35	36 0 36	108908.082	108908.092(18)
37 1 37	38 0 38	62311.483	62311.474(11)
39 1 39	40 0 40	15475.45	15475.415(11)
41 0 41	40 1 40	8030.85	8030.824(11)
42 0 42	41 1 41	31595.01	31594.997(10)
44 0 44	43 1 43	78894.446	78894.452(11)
45 0 45	44 1 44	102628.354	102628.355(17)

[a] The estimated experimental uncertainty in the measured transitions are: for the microwave transitions quoted to two decimal places ≤ ± 0.100 MHz, for millimeter wave transitions above 37 GHz quoted to two decimal places < ± 0.150 MHz, and for those quoted to three decimal places < ± 0.030 MHz.

[b] Note that one standard deviation is presented for the calculated uncertainty. These values should be multiplied by a factor of 2 to obtain ∿ 95 % confidence level.

TABLE 10. Microwave transitions of $H^{14}N^{12}C^{16}O$ in order of frequency

Transition						Frequency (MHz)
1	1	0	1	1	1	160.432
2	1	1	2	1	2	481.293
3	1	2	3	1	3	962.576
4	1	3	4	1	4	1604.270
5	1	4	5	1	5	2406.361
6	1	5	6	1	6	3368.830
7	1	6	7	1	7	4491.659
8	1	7	8	1	8	5774.822
9	1	8	9	1	9	7218.291
10	1	9	10	1	10	8822.034
11	1	10	11	1	11	10586.015
37	1	37	38	0	38	11191.630
12	1	11	12	1	12	12510.196
39	0	39	38	1	38	13665.987
13	1	12	13	1	13	14594.535
14	1	13	14	1	14	16838.985
15	1	14	15	1	15	19243.496
16	1	15	16	1	16	21808.016
1	0	1	0	0	0	21981.574
17	1	16	17	1	17	24532.487
18	1	17	18	1	18	27416.848
19	1	18	19	1	19	30461.036
20	1	19	20	1	20	33664.981
36	1	36	37	0	37	35983.693
21	1	20	21	1	21	37028.612
40	0	40	39	1	39	38588.383
22	1	21	22	1	22	40551.853
2	1	2	1	1	1	43799.019
2	0	2	1	0	1	43963.042
2	1	1	1	1	0	44119.879
23	1	22	23	1	23	44234.625
24	1	23	24	1	24	48076.844
25	1	24	25	1	25	52078.422
35	1	35	36	0	36	60709.448
41	0	41	40	1	40	63574.773
3	1	3	2	1	2	65698.308
3	2	2	2	2	1	65924.118
3	2	1	2	2	0	65924.199
3	0	3	2	0	2	65944.298
3	1	2	2	1	1	66179.590
34	1	34	35	0	35	85368.158
4	1	4	3	1	3	87597.333
4	3	1	3	3	0	87867.280
4	3	2	3	3	1	87867.280
4	2	3	3	2	2	87898.416
4	2	2	3	2	1	87898.620
4	0	4	3	0	3	87925.238
4	1	3	3	1	2	88239.027
42	0	42	41	1	41	88624.352
5	1	5	4	1	4	109496.007
5	4	2	4	4	1	109778.700
5	4	1	4	4	0	109778.700
5	3	2	4	3	1	109833.489
5	3	3	4	3	2	109833.489

TABLE 10—Continued

5	2	4	4	2	3	109872.366
5	2	3	4	2	2	109872.773
5	0	5	4	0	4	109905.753
33	1	33	34	0	34	109959.100
5	1	4	4	1	3	110298.098
43	0	43	42	1	42	113736.298
6	1	6	5	1	5	131394.241
6	5	2	5	5	1	131640.747
6	5	1	5	5	0	131640.747
6	4	2	5	4	1	131733.534
6	4	3	5	4	2	131733.534
6	3	3	5	3	2	131799.292
6	3	4	5	3	3	131799.292
6	2	5	5	2	4	131845.880
6	2	4	5	2	3	131846.590
6	0	6	5	0	5	131885.740
6	1	5	5	1	4	132356.711
32	1	32	33	0	33	134481.571
44	0	44	43	1	43	138909.772
7	1	7	6	1	6	153291.946
7	5	3	6	5	2	153579.619
7	5	2	6	5	1	153579.619
7	4	3	6	4	2	153687.873
7	4	4	6	4	3	153687.873
7	3	4	6	3	3	153764.606
7	3	5	6	3	4	153764.606
7	2	6	6	2	5	153818.869
7	2	5	6	2	4	153820.007
7	0	7	6	0	6	153865.092
7	1	6	6	1	5	154414.776
31	1	31	32	0	32	158934.883
45	0	45	44	1	44	164143.924
8	1	8	7	1	7	175189.037
8	5	4	7	5	3	175517.913
8	5	3	7	5	2	175517.913
8	4	4	7	4	3	175641.637
8	4	5	7	4	4	175641.637
8	3	6	7	3	5	175729.350
8	3	5	7	3	4	175729.351
8	2	7	7	2	6	175791.248
8	2	6	7	2	5	175792.954
8	0	8	7	0	7	175843.703
8	1	7	7	1	6	176472.199
30	1	30	31	0	31	183319.365
46	0	46	45	1	45	189437.882
9	1	9	8	1	8	197085.424
9	5	5	8	5	4	197455.547
9	5	4	8	5	3	197455.547
9	4	5	8	4	4	197594.741
9	4	6	8	4	5	197594.741
9	3	7	8	3	6	197693.444
9	3	6	8	3	5	197693.444

TABLE 10—Continued

9	2	8	8	2	7	197762.928
9	2	7	8	2	6	197765.366
9	0	9	8	0	8	197821.469
9	1	8	8	1	7	198528.892
29	1	29	30	0	30	207631.365
47	0	47	46	1	46	214790.761
10	1	10	9	1	9	218981.019
10	5	6	9	5	5	219392.437
10	5	5	9	5	4	219392.437
10	4	6	9	4	5	219547.105
10	4	7	9	4	6	219547.105
10	3	8	9	3	7	219656.805
10	3	7	9	3	6	219656.805
10	2	9	9	2	8	219733.824
10	2	8	9	2	7	219737.175
10	0	10	9	0	9	219798.282
10	1	9	9	1	8	220584.762
28	1	28	29	0	29	231873.247
11	1	11	10	1	10	240875.735
11	3	9	10	3	8	241619.351
11	3	8	10	3	7	241619.353
11	2	10	10	2	9	241703.846
11	2	9	10	2	8	241708.315
11	0	11	10	0	10	241774.037
11	1	10	10	1	9	242639.717
27	1	27	28	0	28	256043.392
12	1	12	11	1	11	262769.484
12	3	10	11	3	9	263581.003
12	3	9	11	3	8	263581.006
12	2	11	11	2	10	263672.909
12	2	10	11	2	9	263678.717
12	0	12	11	0	11	263748.630
12	1	11	11	1	10	264693.665
26	1	26	27	0	27	280141.198
13	1	13	12	1	12	284662.177
13	3	11	12	3	10	285541.677
13	3	10	12	3	9	285541.681
13	2	12	12	2	11	285640.924
13	2	11	12	2	10	285648.316
13	0	13	12	0	12	285721.952
13	1	12	12	1	11	286746.515
1	1	0	1	0	1	901799.903(0.135)
2	1	1	2	0	2	901956.740(0.133)
3	1	2	3	0	3	902192.032(0.131)
4	1	3	4	0	4	902505.821(0.128)
5	1	4	5	0	5	902898.166(0.125)
6	1	5	6	0	6	903369.137(0.121)
7	1	6	7	0	7	903918.820(0.116)
8	1	7	8	0	8	904547.316(0.111)
9	1	8	9	0	9	905254.739(0.105)
10	1	9	10	0	10	906041.219(0.099)