Ground State Centrifugal Distortion Constants of Vinyl Isocyanide, CH_2-CH-NC, from the Microwave and Millimeter Wave Rotational Spectra *

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The pure rotational spectrum of vinyl isocyanide in the ground vibrational state has been assigned in the frequency region from 8 GHz to 180 GHz. The measured absorption lines encompass 157 a-type transitions from the ^qR_K, $^qQ_1$, $^qQ_2$, $^qQ_3$, $^qQ_4$, and $^qQ_5$ branches and 48 b-type transitions from the $^rP_0$, $^rP_1$, $^rP_2$, $^rP_3$, $^rP_4$, $^rP_5$, $^rQ_0$, and $^rQ_1$ branches for values of J up to 54. The rotational constants have been refined and all quartic and sextic centrifugal distortion constants have been determined using Watson's reduced Hamiltonian. No quadrupole hyperfine splitting was observed.

I. Introduction

Very recently the transition $2_{11} - 2_{12}$ of vinyl cyanide has been detected in interstellar space by Gardner and Winnewisser [1] on the basis of precise predictions of its rotational spectrum in the microwave and millimeter wave region [2]. From optical and radioastronomical observations we know at present that the chemistry which takes place in the cool, dense, interstellar clouds produces other nitriles such as the CN-radical, hydrogen cyanide ($HC \equiv N$), cyanoacetylene ($HC \equiv C - C \equiv N$) and methylcyanide ($H_3C - C \equiv N$) [3]. However, there is so far no experimental evidence that the corresponding isonitriles can be synthesised under interstellar space conditions, despite the suspicion that the unidentified line U(90665) might arise from the HNC molecule [4], whose laboratory spectrum has yet to be discovered. The presence of vinyl isocyanide ($V - NC$) in interstellar space, however, is more probable than that of smaller isonitriles, since it is relatively stable. The a-type rotational transitions of this molecule are very intense because of the large a-component of its dipole moment ($\mu_a = 3.47$ D and $\mu_b = 0.79$ D [5]), so that we consider $V - NC$ a good candidate for detection in interstellar clouds.

The rotational constants of vinyl isocyanide for molecules in the ground state and in the two lowest excited vibrational states were reported by Bolton, Owen and Sheridan [5]. They measured several low J a-type transitions and four b-type, $K_a = 1 \leftarrow 0$, transitions in the ground state. They also reported the vibrational frequencies of 15 fundamentals and several combination and overtone bands.

The purpose of the present work is to extend the measurements of the rotational spectrum into the millimeter wave region in order to refine the rotational constants and to determine the quartic and sextic distortion constants. A large number of both a- and b-type transitions have been identified up to $J = 54$ for the ground vibrational state. The observed frequencies have been analysed by the centrifugal distortion treatment using J^6 terms in the Hamiltonian.

Precise predictions of line frequencies have been made for radioastronomically interesting transitions of this molecule on the basis of the adjusted molecular parameters derived from the experimental data reported here.

The notation used in this paper is the same as that used by Watson [6] and by Kivelson and Wilson [7].

II. Experimental Procedures

The sample of vinyl isocyanide was prepared following the method reported by Matteson and Bailey [8]. In the first step, N-formylethanolamine was prepared by the dropwise addition of ethyl formate to ethanolamine. The product was distilled at about 130° under a vacuum of less than 1 torr. In the next step, 2-isocyanoethyl benzenesulfonate was obtained by the dropwise addition of benzenesulfonyl chloride

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to N-formyl-ethanolamine in pyridine under a nitrogen atmosphere. The product was extracted with methylene chloride and concentrated under vacuum.

$$\begin{array}{l} HOCH_2CH_2NH_2 \\ \quad + \quad \rightarrow HOCH_2CH_2NHCHO \\ EtOCHO \qquad\qquad + \\ \qquad\qquad\quad C_6H_5SO_2Cl \end{array}$$

Finally vinyl isocyanide was obtained by adding potassium hydroxide in ethanol to the ethanol solution of crude 2-isocyanoethyl benzenesulfonate.

$$\rightarrow C_6H_5SO_2OCH_2CH_2NC \rightarrow CH_2CH-NC$$

The product was purified by a fractionation at about -50° C. Finally V – NC was sublimed at dry ice temperature into the cells of the spectrometers. No obvious impurity has been found in the spectrum other than the solvent methylene chloride.

Microwave measurements were carried out in the frequency region 8 – 18 GHz, using a Hewlett-Packard MODEL 8460 A Microwave Rotational Resonance (MRR) spectrometer employing a 6 foot X-band Stark cell and 33.333 kHz square wave modulation of the electric field. The reproducibility of the measurements in the present study obtained by averaging the center frequencies of the forward and reverse sweeps through the absorption line profile is believed to be better than ± 20 kHz.

In the spectral region of 70 – 180 GHz, a millimeter wave spectrometer was used with a three meter free space absorption cell. The use of an on-line PDP 8/I minicomputer for signal averaging and data processing with the spectrometer has been described previously [9]. The accuracy of the measurements with this spectrometer is believed to be better than ± 10 kHz, except for very weak lines or overlapping lines [10].

The spectra were observed and measured at room temperature. All measurements were made at sample pressures less than 10^{-2} torr.

III. Spectra and Assignment

A general view of the rotational spectrum arising from *a*-type transitions is shown in the Fortrat diagram of Fig. 1 and the spectrum produced by the *b*-ytpe transitions is shown in Figure 2. The solid circles represent observed lines and the open circles represent predicted line positions. The *a*-type R branch transitions, corresponding to $\Delta J = 1$ and $\Delta K_a = 0$ transitions, are indicated by showing only the $K_a = 1$ lines. The actual pattern of each such group of transitions is illustrated by a plot of the transition $J = 14 \leftarrow 13$ in Figure 3. The band-head at $K_a = 5$ is caused by the superposition of centrifugal distortion contributions from terms with Δ_J and Δ_{JK}. This type of band-head is typical for slightly asymmetric-top molecules and helps in the assignment of the millimeter wave spectrum, since the band-heads form characteristic groups of lines which are spaced by (B + C). The band-head structure of vinyl isocyanide, vinyl cyanide [2], propynal [11] and acrolein [12] are compared in Figure 4. The pattern of the transitions from vinyl isocyanide is quite similar to that of vinyl cyanide.

The other band-head at $K_a = 2$ is caused by the inertial asymmetry of the molecule. It is easily seen that the inertial asymmetry of propynal is less than that of the other molecules in Figure 4. Since the inertial asymmetry of vinyl isocyanide $\varkappa = -0.977786$ or $b_p = -5.58457 \times 10^{-5}$ is fairly large, the *K*-type doublet of $K_a = 4$ could be resolved for $J \geqq 10$.

The *a*-type Q branch transitions, which are transitions between the *K*-type doublets for $K_a = 1, 2, 3, 4$

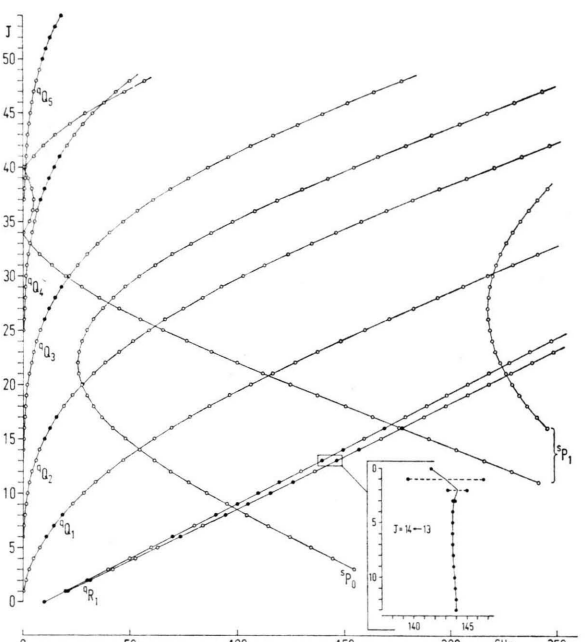

Fig. 1. Fortrat-diagram for a-type transitions of V-NC. The solid and open circles indicate measured and predicted line positions, respectively. For the a-type R branch only the $K_a = 1$ transitions are indicated ($K_a = 0$ for $J = 1 \leftarrow 0$). The inset shows the full K_a-pattern for one transition.

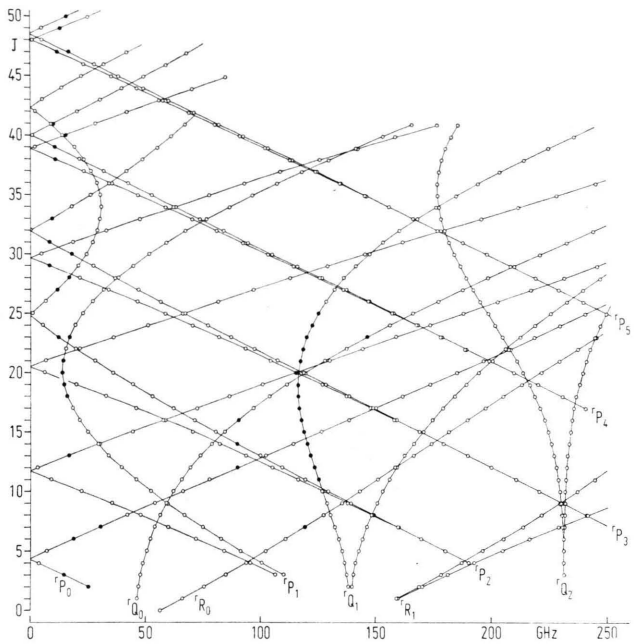

Fig. 2. Fortrat-diagram for the *b*-type transitions of V-NC. The solid and open circles indicate measured and predicted line positions, respectively.

and 5, supply information concerning high J states and therefore are important in determining several of the distortion constants.

The *b*-type transitions shown in Fig. 2 also exhibit band-head structure, which is caused primarily by the inertial asymmetry contribution. Fortunately one component of the *b*-type P branch transitions, $J-1 \leftarrow J$ and $K_a = 2 \leftarrow 1$, forms a band-head in the frequency range of our MRR spectrometer. These band-head lines contributed significantly to the determination of the Δ_K centrifugal distortion constant.

The assignment of the lines was achieved by a bootstrap procedure. Initially the spectrum was predicted using the previously reported rotational constants [5] and the centrifugal distortion constants of vinyl cyanide [2]. The *a*-type R branch transitions were identified in the millimeter wave region by their characteristic band-head structures mentioned above. The band heads were predicted adequately with the assumed constants. Refined molecular constants were used to predict further transition frequencies. The absorption lines in the 8 – 18 GHz region belonging to *a*-type and to *b*-type transitions could then be identified. Assignments in the 8 – 18 GHz region were confirmed by the Stark patterns. Relative intensity also helped the assignment; otherwise the frequency fit was the chief criterion for the assignment. Further *b*-type transitions were then assigned in the mm-wave region.

In this way 157 *a*-type transitions from ^qR_K, $^qQ_1$, $^qQ_2$, $^qQ_3$, $^qQ_4$, and $^qQ_5$ branches and 48 *b*-type transitions from the $^rP_0$, $^rP_1$, $^rP_2$, $^rP_3$, $^rP_4$, $^rP_5$, $^rQ_0$, and $^rQ_1$ branches for values of J up to 54 have been identified including the previously reported lines. Some of the lines reported earlier were remeasured in the present study. Because of the fairly small *b*-component of the dipole moment the line intensity of *b*-type transitions is much weaker than that of *a*-type transitions. However, the weak *b*-type transitions in the millimeter wave region were measured accurately with the aid of the signal averaging system described in Reference [10]. The averaged and smoothed line profile of a *b*-type transition is illustrated in Figure 5.

It should be mentioned that it is impractical to attempt to measure all *b*-type or *a*-type transition in

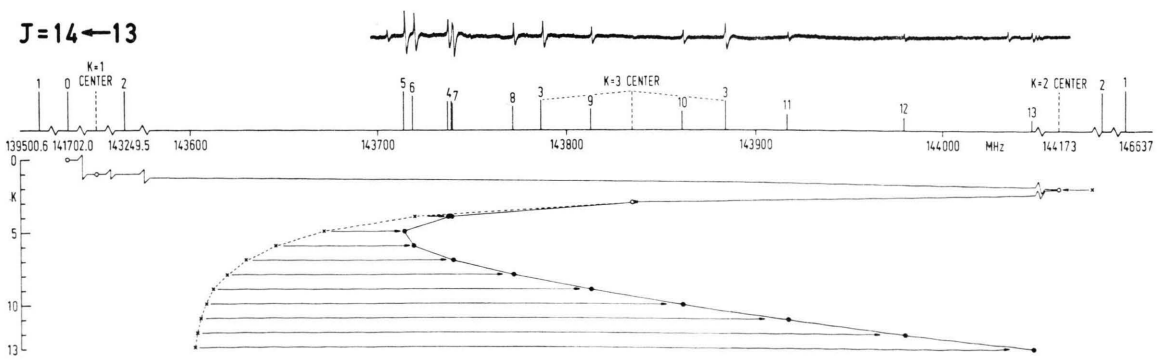

Fig. 3. Oscilloscope display of the a-type $J = 14 \leftarrow 13$ transition of vinyl isocyanide showing the band-head structure. Deviation from rigid rotor frequencies due to centrifugal distortion is indicated by arrows. The weak lines at the tail of the series are believed to arise from molecules in excited vibrational states.

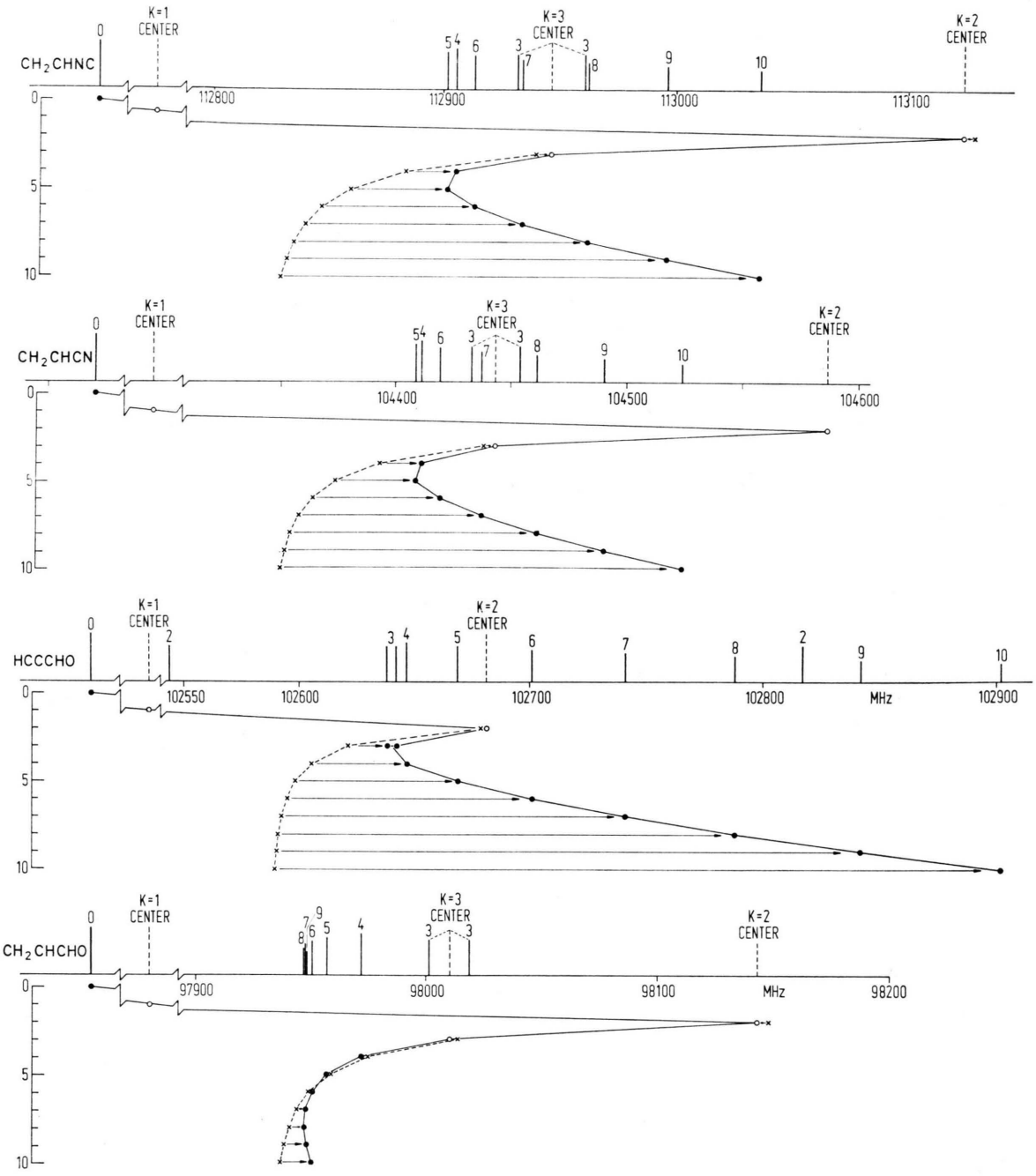

Fig. 4. The band-head structure in the spectrum of several slightly asymmetric (near prolate) top molecules are illustrated for the a-type $J=11 \leftarrow 10$ transition. Deviation from the rigid rotor pattern due to centrifugal distortion is indicated by arrows.

the frequency region $0-200$ GHz which can be expected to have reasonable intensity. Our approach has been to measure transitions of various branches belonging to as many K subbands as possible. These transitions yielded reliable spectroscopic parameters which may be used to predict the remainder of the spectrum.

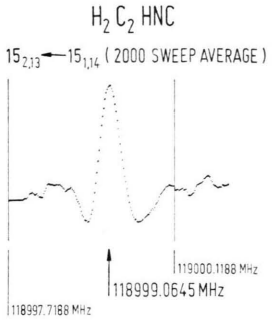

Fig. 5. Oscilloscope display of the b-type $15_{2,13} \leftarrow 15_{1,14}$ transition of V-NC after 2000 sweeps and 25 point parabolic smoothing.

IV. Hamiltonian and Analysis

The observed rotational transitions have been analysed by the use of the reduced Hamiltonian reported by Watson [6], in which $R_6 = 0$,

$$\begin{aligned}\mathcal{H} = {} & \tfrac{1}{2}(X+Y)J^2 + \{Z - \tfrac{1}{2}(X+Y)\}J_z^2 \\ & - \Delta_J (J^2)^2 - \Delta_{JK} J^2 J_z^2 - \Delta_K J_z^4 \\ & + H_J (J^2)^3 + H_{JK}(J^2)^2 J_z^2 + H_{KJ} J^2 J_z^4 + H_K J_z^6 \\ & + (J_x^2 - J_y^2)\{\tfrac{1}{4}(X-Y) - \delta_J J^2 - \delta_K J_z^2 \\ & + h_J (J^2)^2 + h_{JK} J^2 J_z^2 + h_K J_z^4\} \\ & + \{\tfrac{1}{4}(X-Y) - \delta_J J^2 - \delta_K J_z^2 \\ & + h_J (J^2)^2 + h_{JK} J^2 J_z^2 + h_K J_z^4\}(J_x^2 - J_y^2)\end{aligned} \tag{1}$$

where J, J_x, J_y, and J_z are the operators for the total angular momentum and its components. The constants, X, Y, and Z, are the Watson's reduced rotational constants $\tilde{B}$, $\tilde{C}$, and $\tilde{A}$, respectively, in the I^r axis representation [13].

The direct diagonalization of the energy matrix has been used to obtain the rotational energy levels with the aid of the QR algorithm [14] which diagonalizes tridiagonal matrices rapidly. The computations were carried out using Fortran IV coded programs and employing double precision arithmetic utilizing 25 decimal digits throughout the energy calculation. The iterative least-squares method has been applied in order to obtain the 15 molecular constants which appear in the above Hamiltonian.

Table I lists the observed and calculated frequencies for 157 a-type transitions and 48 b-type transitions together with astrophysically important line frequency predictions. Two b-type transitions, $1_{11} \leftarrow 2_{02}$ and $6_{16} \leftarrow 7_{07}$, reported in Ref. [5] have been included in the least-squares fit although the other lines reported in Ref. [5] were rejected from the fit. We included these two lines because we could measure only two other transitions which belong to the $^rP_0$ branch. For the other branches we were able to measure enough transitions. Several lines were rejected from the fit, indicating an error in measurement, and several high K_a lines were omitted from the fit because higher order centrifugal distortion effects appear to contribute to those line frequencies. Accidentally overlapped or partially resolved K-type doublets are also omitted. The K-type doublets in the a-type R branch transitions are considered to be a single line when the calculated splitting is less than 5 kHz. Thus 173 lines out of 205 measured transitions have been used for the least-squares analysis and the standard deviation of the fit was obtained to be 19.5 kHz, which corresponds to the assumed reproducibility of the frequency measurements.

The constants obtained in the I^r axis representation [13] are listed in Table II. The rotational and quartic centrifugal distortion constants are well determined. For the sextic centrifugal distortion constants, the standard errors are on the order of 10% of the values of the constants.

V. Discussion

a) Molecular Parameters

The determinable parameters found by Watson [6] which are invariant to a unitary transformation of the Hamiltonian, $\mathfrak{A}$, $\mathfrak{B}$, $\mathfrak{C}$, τ'_{aaaa}, τ'_{bbbb}, τ'_{cccc}, τ_1, and τ_2, are listed in Table III. Following the planarity condition derived by Watson [6], the quantity known as τ-defect,

$$\Delta\tau'_{cccc} = \tau'_{cccc} - \frac{1}{\mathfrak{A}+\mathfrak{B}}(\tau_2 - \mathfrak{C}\tau_1) \tag{2}$$

should be zero for the equilibrium structure of a planar molecule. For the ground vibrational state of the V−NC molecule the τ-defect obtained from Eq. (2) is 133 kHz, caused by vibrational effects. Introducing the planarity conditions among the τ's,

$$\tau_{aabb} = \tfrac{1}{2}A^2B^2\left\{-\frac{\tau_{aaaa}}{A^4} - \frac{\tau_{bbbb}}{B^4} + \frac{\tau_{cccc}}{C^4}\right\}, \tag{3}$$

$$\tau_{bbcc} = \tfrac{1}{2}B^2C^2\left\{-\frac{\tau_{aaaa}}{A^4} + \frac{\tau_{bbbb}}{B^4} + \frac{\tau_{cccc}}{C^4}\right\}, \tag{4}$$

and

$$\tau_{ccaa} = \tfrac{1}{2}A^2C^2\left\{-\frac{\tau_{aaaa}}{A^4} - \frac{\tau_{bbbb}}{B^4} + \frac{\tau_{cccc}}{C^4}\right\} \tag{5}$$

TABLE I. OBSERVED AND CALCULATED FREQUENCIES OF VINYL ISOCYANIDE IN MHz (CONTINUED)

TRANSITION UPPER STATE	TRANSITION LOWER STATE	OBSERVED FREQUENCY (WEIGHT)	CALCULATED FREQUENCY (STANDARD DEVIATION)	OBS.-CALC.	ENERGY LEVELS IN CM-1 UPPER STATE	ENERGY LEVELS IN CM-1 LOWER STATE	REMARKS
7(5, 3) -	6(5, 2)	71836.0854(1.0)	71836.0846(0.0024)	0.0008	48.166	45.770	
7(6, 1) -	6(6, 0)		71848.2376(0.0026)		65.099	62.702	
7(6, 2) -	6(6, 1)	71848.2201(1.0)	71848.2375(0.0126)	-0.0175	65.099	62.702	
8(0, 8) -	7(0, 7)		81678.4555(0.0034)		12.285	9.560	
8(1, 7) -	7(1, 6)		84021.1049(0.0034)		14.165	11.362	
8(1, 8) -	7(1, 7)		79888.2568(0.0034)		13.544	10.879	
8(2, 6) -	7(2, 5)		82354.3907(0.0032)		18.525	15.778	
8(2, 7) -	7(2, 6)		81993.2379(0.0032)		18.494	15.759	
8(3, 5) -	7(3, 4)		82108.9387(0.0029)		26.228	23.489	
8(3, 6) -	7(3, 5)		82103.2358(0.0029)		26.227	23.489	
8(4, 4) -	7(4, 3)		82095.6931(0.0026)		37.030	34.292	
8(4, 5) -	7(4, 4)		82095.6607(0.0026)		37.030	34.292	
8(5, 3) -	7(5, 2)		82100.8123(0.0025)		50.904	48.166	
8(5, 4) -	7(5, 3)		82100.8122(0.0025)		50.904	48.166	
8(6, 2) -	7(6, 1)		82113.5633(0.0028)		67.838	65.099	
8(6, 3) -	7(6, 2)		82113.5633(0.0028)		67.838	65.099	
8(7, 1) -	7(7, 0)		82131.5200(0.0035)		87.815	85.075	
8(7, 2) -	7(7, 1)		82131.5200(0.0035)		87.815	85.075	
9(0, 9) -	8(0, 8)	91779.3754(1.0)	91779.3717(0.0035)	0.0037	15.346	12.285	
9(1, 8) -	8(1, 7)	94492.3183(1.0)	94492.2981(0.0035)	0.0202	17.317	14.165	
9(1, 9) -	8(1, 8)	89847.5611(1.0)	89847.5442(0.0035)	0.0169	16.541	13.544	
9(2, 7) -	8(2, 6)	92736.1904(1.0)	92736.1828(0.0033)	0.0076	21.618	18.525	
9(2, 8) -	8(2, 7)	92222.5603(1.0)	92222.5508(0.0033)	0.0095	21.571	18.494	
9(3, 6) -	8(3, 5)	92386.9085(1.0)	92386.8974(0.0030)	0.0111	29.309	26.228	
9(3, 7) -	8(3, 6)	92376.4663(1.0)	92376.4527(0.0029)	0.0136	29.309	26.227	
9(4, 5) -	8(4, 4)	92363.4893(1.0)	92363.5363(0.0027)	-0.0470	40.111	37.030	b
9(4, 6) -	8(4, 5)	92363.4893(1.0)	92363.4585(0.0027)	0.0308	40.111	37.030	b
9(5, 4) -	8(5, 3)		92366.5102(0.0026)		53.986	50.904	
9(5, 5) -	8(5, 4)	92366.5009(1.0)	92366.5099(0.0026)	-0.0090	53.986	50.904	
9(6, 3) -	8(6, 2)		92379.4044(0.0029)		70.919	67.838	
9(6, 4) -	8(6, 3)	92379.4039(1.0)	92379.4044(0.0029)	-0.0005	70.919	67.838	
9(7, 2) -	8(7, 1)		92398.7453(0.0036)		90.897	87.815	
9(7, 3) -	8(7, 2)	92398.7376(1.0)	92398.7453(0.0036)	-0.0077	90.897	87.815	
9(8, 1) -	8(8, 0)		92423.1909(0.0046)		113.901	110.818	
9(8, 2) -	8(8, 1)	92423.1974(1.0)	92423.1909(0.0046)	0.0065	113.901	110.818	
10(0,10) -	9(0, 9)	101843.8299(1.0)	101843.8659(0.0036)	-0.0360	18.743	15.346	
10(1, 9) -	9(1, 8)	104951.7225(1.0)	104951.7539(0.0035)	-0.0314	20.817	17.317	
10(1,10) -	9(1, 9)		99798.0262(0.0035)		19.869	16.541	
10(2, 8) -	9(2, 7)	103146.8133(1.0)	103146.8409(0.0033)	-0.0276	25.059	21.618	
10(2, 9) -	9(2, 8)	102444.8694(1.0)	102444.8870(0.0033)	-0.0176	24.988	21.571	
10(3, 7) -	9(3, 6)	102670.5602(1.0)	102670.5671(0.0030)	-0.0069	32.734	29.309	
10(3, 8) -	9(3, 7)	102652.6915(1.0)	102652.6852(0.0030)	0.0063	32.733	29.309	
10(4, 6) -	9(4, 5)	102633.3628(0.0)	102633.4681(0.0027)	-0.1053	43.535	40.111	c
10(4, 7) -	9(4, 6)	102633.3628(0.0)	102633.2997(0.0027)	0.0631	43.535	40.111	c
10(5, 5) -	9(5, 4)		102633.2985(0.0027)		57.409	53.986	
10(5, 6) -	9(5, 5)	102633.3628(0.0)	102633.2978(0.0027)	0.0650	57.409	53.986	c
10(6, 4) -	9(6, 3)		102645.8245(0.0030)		74.343	70.919	
10(6, 5) -	9(6, 4)	102645.8054(1.0)	102645.8245(0.0030)	-0.0191	74.343	70.919	
10(7, 3) -	9(7, 2)		102666.2465(0.0037)		94.321	90.897	
10(7, 4) -	9(7, 3)	102666.2437(1.0)	102666.2465(0.0037)	-0.0028	94.321	90.897	
10(8, 2) -	9(8, 1)		102692.7194(0.0047)		117.326	113.901	
10(8, 3) -	9(8, 2)	102692.7130(1.0)	102692.7194(0.0047)	-0.0064	117.326	113.901	

TABLE I. OBSERVED AND CALCULATED FREQUENCIES OF VINYL ISOCYANIDE IN MHz

TRANSITION UPPER STATE	TRANSITION LOWER STATE	OBSERVED FREQUENCY (WEIGHT)	CALCULATED FREQUENCY (STANDARD DEVIATION)	OBS.-CALC.	ENERGY LEVELS IN CM-1 UPPER STATE	ENERGY LEVELS IN CM-1 LOWER STATE	REMARKS
** A TYPE R BRANCH **							
1(0, 1) -	0(0, 0)	10255.5810(1.0)	10255.5789(0.0006)	0.0021	0.342	0.000	
2(0, 2) -	1(0, 1)	20506.7800(0.0)	20506.7643(0.0011)	0.0157	1.026	0.342	a
2(1, 1) -	1(1, 0)	21029.0400(0.0)	21029.0805(0.0012)	-0.0405	2.598	1.897	a
2(1, 2) -	1(1, 1)	19993.9800(0.0)	19993.9162(0.0011)	0.0638	2.546	1.879	a
3(0, 3) -	2(0, 2)	30749.0300(0.0)	30749.1661(0.0017)	-0.1361	2.052	1.026	a
3(1, 2) -	2(1, 1)	31540.6900(0.0)	31540.7214(0.0017)	-0.0314	3.650	2.598	a
3(1, 3) -	2(1, 2)	29988.0500(0.0)	29988.0634(0.0016)	-0.0134	3.547	2.546	a
3(2, 1) -	2(2, 0)	30786.4100(0.0)	30786.2321(0.0016)	0.1779	8.236	7.209	a
3(2, 2) -	2(2, 1)	30768.9600(0.0)	30768.8993(0.0016)	0.0607	8.235	7.209	a
4(0, 4) -	3(0, 3)		40978.4074(0.0022)		3.419	2.052	
4(1, 3) -	3(1, 2)		42048.8521(0.0022)		5.053	3.650	
4(1, 4) -	3(1, 3)		39978.8702(0.0021)		4.880	3.547	
4(2, 2) -	3(2, 1)		41064.8719(0.0020)		9.606	8.236	
4(2, 3) -	3(2, 2)		41021.5581(0.0020)		9.604	8.235	
4(3, 1) -	3(3, 0)		41037.6516(0.0018)		17.328	15.959	
4(3, 2) -	3(3, 1)		41037.5155(0.0018)		17.328	15.959	
5(0, 5) -	4(0, 4)		51190.1460(0.0026)		5.126	3.419	
5(1, 4) -	4(1, 3)		52552.2511(0.0026)		6.806	5.053	
5(1, 5) -	4(1, 4)		49965.2772(0.0025)		6.547	4.880	
5(2, 3) -	4(2, 2)		51357.6569(0.0024)		11.319	9.606	
5(2, 4) -	4(2, 3)		51271.0977(0.0024)		11.314	9.604	
5(3, 2) -	4(3, 1)		51300.8410(0.0022)		19.039	17.328	
5(3, 3) -	4(3, 2)		51300.3649(0.0022)		19.039	17.328	
5(4, 1) -	4(4, 0)		51302.3232(0.0020)		29.842	28.131	
5(4, 2) -	4(4, 1)		51302.3224(0.0020)		29.842	28.131	
6(0, 6) -	5(0, 5)		61380.1147(0.0030)		7.174	5.126	
6(1, 5) -	5(1, 4)		63049.6522(0.0030)		8.909	6.806	
6(1, 6) -	5(1, 5)		59946.2709(0.0029)		8.546	6.547	
6(2, 4) -	5(2, 3)		61668.0161(0.0027)		13.376	11.319	
6(2, 5) -	5(2, 4)		61516.7407(0.0027)		13.366	11.314	
6(3, 3) -	5(3, 2)		61566.6720(0.0025)		21.093	19.039	
6(3, 4) -	5(3, 3)		61555.4030(0.0025)		21.093	19.039	
6(4, 2) -	5(4, 1)		61565.3203(0.0023)		31.896	29.842	
6(4, 3) -	5(4, 2)		61565.3167(0.0023)		31.896	29.842	
6(5, 1) -	5(5, 0)		61572.2065(0.0022)		45.770	43.716	
6(5, 2) -	5(5, 1)		61572.2065(0.0022)		45.770	43.716	
7(0, 7) -	6(0, 6)	71544.1836(1.0)	71544.1848(0.0032)	-0.0012	9.560	7.174	
7(1, 6) -	6(1, 5)	73539.7509(1.0)	73539.7333(0.0032)	0.0176	11.362	8.909	
7(1, 7) -	6(1, 6)	69920.8973(1.0)	69920.8943(0.0032)	0.0030	10.879	8.546	
7(2, 5) -	6(2, 4)	71999.2179(1.0)	71999.2400(0.0030)	-0.0221	15.778	13.376	
7(2, 6) -	6(2, 5)	71757.7418(1.0)	71757.7117(0.0030)	0.0301	15.759	13.366	
7(3, 4) -	6(3, 3)	71835.7886(1.0)	71835.7974(0.0027)	-0.0088	23.489	21.093	
7(3, 5) -	6(3, 4)	71832.9480(1.0)	71832.9438(0.0027)	0.0042	23.489	21.093	
7(4, 4) -	6(4, 3)	71829.6988(1.0)	71829.6876(0.0025)	0.0112	34.292	31.896	
7(4, 3) -	6(4, 2)	71829.6988(1.0)	71829.6994(0.0025)	-0.0006	34.292	31.896	
7(5, 2) -	6(5, 1)		71836.0846(0.0024)		48.166	45.770	

TABLE I. OBSERVED AND CALCULATED FREQUENCIES OF VINYL ISOCYANIDE IN MHz (CONTINUED)

TRANSITION UPPER STATE	TRANSITION LOWER STATE	OBSERVED FREQUENCY (WEIGHT)	CALCULATED FREQUENCY (STANDARD DEVIATION)	OBS.-CALC.	ENERGY LEVELS IN CM-1 UPPER STATE	ENERGY LEVELS IN CM-1 LOWER STATE	REMARKS
10(9, 1) -	9(9, 0)		102724.4037(0.0058)		143.338	139.911	
10(9, 2) -	9(9, 1)	102724.3949(1.0)	102724.4037(0.0058)	-0.0088	143.338	139.911	
11(0,11) -	10(0,10)	111869.4900(1.0)	111869.5154(0.0036)	-0.0254	22.475	18.743	
11(1,10) -	10(1, 9)	115397.8455(1.0)	115397.8119(0.0035)	0.0336	24.667	20.817	
11(1,11) -	10(1,10)	109739.1063(0.0)	109739.0644(0.0035)	0.0419	23.530	19.869	e
11(2, 9) -	10(2, 8)	113588.0381(0.0)	113587.9399(0.0033)	0.0982	28.848	25.059	e
11(2,10) -	10(2, 9)	112659.5123(1.0)	112659.4901(0.0033)	0.0222	28.746	24.988	
11(3, 8) -	10(3, 7)	112960.3940(1.0)	112960.9437(0.0029)	0.0503	36.502	32.734	
11(3, 9) -	10(3, 8)	112931.9415(1.0)	112931.9339(0.0029)	0.0076	36.500	32.733	
11(4, 7) -	10(4, 6)	112905.7263(0.0)	112905.7335(0.0027)	-0.0072	47.301	43.535	d
11(4, 8) -	10(4, 7)	112905.4966(0.0)	112905.3969(0.0027)	0.0997	47.301	43.535	d
11(5, 6) -	10(5, 5)		112901.2974(0.0027)		61.175	57.409	
11(5, 7) -	10(5, 6)	112901.3182(1.0)	112901.2955(0.0027)	0.0227	61.175	57.409	
11(6, 5) -	10(6, 4)		112912.8870(0.0030)		78.109	74.343	
11(6, 6) -	10(6, 5)	112912.8597(1.0)	112912.8870(0.0030)	-0.0273	78.109	74.343	
11(7, 4) -	10(7, 3)		112934.0535(0.0037)		98.088	94.321	
11(7, 5) -	10(7, 4)	112934.0459(1.0)	112934.0536(0.0037)	-0.0077	98.088	94.321	
11(8, 3) -	10(8, 2)		112962.3368(0.0046)		121.094	117.326	
11(8, 4) -	10(8, 3)	112962.3771(1.0)	112962.3368(0.0046)	0.0403	121.094	117.326	
11(9, 2) -	10(9, 1)		112996.6151(0.0057)		147.107	143.338	
11(9, 3) -	10(9, 2)	112996.6478(1.0)	112996.6151(0.0057)	0.0327	147.107	143.338	
11(10, 1) -	10(10, 0)		113036.3240(0.0070)		176.104	172.333	
11(10, 2) -	10(10, 1)	113036.2870(0.0)	113036.3240(0.0070)	-0.0370	176.104	172.333	e
12(0,12) -	11(0,11)	121854.7042(1.0)	121854.7003(0.0035)	0.0039	26.539	22.475	
12(1,11) -	11(1,10)	125828.7008(1.0)	125828.7003(0.0035)	0.0005	28.864	24.667	
12(1,12) -	11(1,11)	119670.1180(1.0)	119670.1179(0.0034)	0.0001	27.522	23.530	
12(2,10) -	11(2, 9)	124060.2454(1.0)	124060.2449(0.0032)	0.0005	32.986	28.848	
12(2,11) -	11(2,10)	122865.5985(1.0)	122865.6128(0.0032)	-0.0143	32.844	28.746	
12(3, 9) -	11(3, 8)	123259.1269(1.0)	123259.1359(0.0029)	-0.0090	40.613	36.502	
12(3,10) -	11(3, 9)	123214.1165(1.0)	123214.1035(0.0029)	0.0130	40.610	36.500	
12(4, 8) -	11(4, 7)	123180.6219(0.0)	123180.5858(0.0026)	0.0361	51.410	47.301	c
12(4, 9) -	11(4, 8)	123179.9323(1.0)	123179.9554(0.0026)	-0.0231	51.409	47.301	
12(5, 7) -	11(5, 6)	123170.6343(1.0)	123170.6268(0.0026)	0.0075	65.283	61.175	
12(5, 8) -	11(5, 7)	123170.6343(1.0)	123170.6224(0.0026)	0.0119	65.283	61.175	
12(6, 6) -	11(6, 5)		123180.6551(0.0030)		82.218	78.109	
12(6, 7) -	11(6, 6)	123180.6219(0.0)	123180.6551(0.0030)	-0.0332	82.218	78.109	c
12(7, 5) -	11(7, 4)		123202.1962(0.0037)		102.198	98.088	
12(7, 6) -	11(7, 5)	123202.1916(1.0)	123202.1962(0.0037)	-0.0046	102.198	98.088	
12(8, 4) -	11(8, 3)		123232.0512(0.0045)		125.205	121.094	
12(8, 5) -	11(8, 4)	123232.0508(1.0)	123232.0512(0.0045)	-0.0004	125.205	121.094	
12(9, 3) -	11(9, 2)		123268.7598(0.0054)		151.219	147.107	
12(9, 4) -	11(9, 3)	123268.7199(1.0)	123268.7598(0.0054)	-0.0399	151.219	147.107	
12(10, 2) -	11(10, 1)		123311.5844(0.0065)		180.217	176.104	
12(10, 3) -	11(10, 2)	123311.5856(1.0)	123311.5844(0.0065)	0.0012	180.217	176.104	
12(11, 1) -	11(11, 0)		123360.1277(0.0080)		212.175	208.060	
12(11, 2) -	11(11, 1)	123360.8568(0.0)	123360.1277(0.0080)	0.7291	212.175	208.060	e
13(0,13) -	12(0,12)		131798.7428(0.0035)		30.936	26.539	
13(1,12) -	12(1,11)		136242.5281(0.0035)		33.408	28.864	
13(1,13) -	12(1,12)		129590.7474(0.0034)		31.844	27.522	
13(2,11) -	12(2,10)		134563.5696(0.0032)		37.474	32.986	

TABLE I. OBSERVED AND CALCULATED FREQUENCIES OF VINYL ISOCYANIDE IN MHz (CONTINUED)

TRANSITION UPPER STATE	TRANSITION LOWER STATE	OBSERVED FREQUENCY (WEIGHT)	CALCULATED FREQUENCY (STANDARD DEVIATION)	OBS.-CALC.	ENERGY LEVELS IN CM-1 UPPER STATE	ENERGY LEVELS IN CM-1 LOWER STATE	REMARKS
13(2,12)	- 12(2,11)		133062.5189(0.0032)		37.283	32.844	
13(3,10)	- 12(3, 9)		133566.3733(0.0028)		45.069	40.613	
13(3,11)	- 12(3,10)		133498.9990(0.0028)		45.063	40.610	
13(4, 9)	- 12(4, 8)		133458.2897(0.0026)		55.861	51.410	
13(4,10)	- 12(4, 9)		133457.1704(0.0026)		55.861	51.409	
13(5, 8)	- 12(5, 7)		133441.4067(0.0026)		69.735	65.283	
13(5, 9)	- 12(5, 8)		133441.3974(0.0026)		69.735	65.283	
13(6, 7)	- 12(6, 6)		133449.1916(0.0031)		86.670	82.218	
13(6, 8)	- 12(6, 7)		133449.1915(0.0031)		86.670	82.218	
13(7, 6)	- 12(7, 5)		133470.7040(0.0037)		106.650	102.198	
13(7, 7)	- 12(7, 6)		133470.7040(0.0037)		106.650	102.198	
13(8, 5)	- 12(8, 4)		133501.8709(0.0044)		129.658	125.205	
13(8, 6)	- 12(8, 5)		133501.8709(0.0044)		129.658	125.205	
13(9, 4)	- 12(9, 3)		133540.8314(0.0050)		155.673	151.219	
13(9, 5)	- 12(9, 4)		133540.8314(0.0050)		155.673	151.219	
13(10, 3)	- 12(10, 2)		133586.6431(0.0058)		184.673	180.217	
13(10, 4)	- 12(10, 3)		133586.6431(0.0058)		184.673	180.217	
13(11, 2)	- 12(11, 1)		133638.7954(0.0070)		216.633	212.175	
13(11, 3)	- 12(11, 2)		133638.7954(0.0070)		216.633	212.175	
13(12, 1)	- 12(12, 0)		133697.0012(0.0092)		251.525	247.065	
13(12, 2)	- 12(12, 1)		133697.0012(0.0092)		251.525	247.065	
14(0,14)	- 13(0,13)	141701.9963(1.0)	141702.0026(0.0035)	-0.0063	35.662	30.936	
14(1,13)	- 13(1,12)	146637.2693(1.0)	146637.2784(0.0036)	-0.0091	38.300	33.408	
14(1,14)	- 13(1,13)	139500.6273(1.0)	139500.6180(0.0034)	0.0093	36.498	31.844	
14(2,12)	- 13(2,11)	145096.6617(1.0)	145096.6765(0.0033)	-0.0148	42.314	37.474	
14(2,13)	- 13(2,12)	143249.4778(1.0)	143249.4866(0.0032)	-0.0088	42.061	37.283	
14(3,11)	- 13(3,10)	143884.0282(1.0)	143884.0125(0.0029)	0.0157	49.868	45.069	
14(3,12)	- 13(3,11)	143786.3327(1.0)	143786.3228(0.0029)	0.0099	49.859	45.063	
14(4,10)	- 13(4, 9)	143739.1009(1.0)	143739.1248(0.0027)	-0.0239	60.656	55.861	
14(4,11)	- 13(4,10)	143737.2459(1.0)	143737.2249(0.0027)	0.0210	60.656	55.861	
14(5, 9)	- 13(5, 8)	143713.7276(1.0)	143713.7574(0.0028)	-0.0298	74.528	69.735	
14(5,10)	- 13(5, 9)	143713.7276(1.0)	143713.7387(0.0028)	-0.0111	74.528	69.735	
14(6, 8)	- 13(6, 7)		143718.5590(0.0032)		91.464	86.670	
14(6, 9)	- 13(6, 8)	143718.5371(1.0)	143718.5589(0.0032)	-0.0218	91.464	86.670	
14(7, 7)	- 13(7, 6)		143739.6063(0.0038)		111.445	106.650	
14(7, 8)	- 13(7, 7)	143739.6230(1.0)	143739.6063(0.0038)	0.0167	111.445	106.650	
14(8, 6)	- 13(8, 5)		143771.8038(0.0043)		134.454	129.658	
14(8, 7)	- 13(8, 6)	143771.7905(1.0)	143771.8038(0.0043)	-0.0133	134.454	129.658	
14(9, 5)	- 13(9, 4)		143812.8232(0.0047)		160.470	155.673	
14(9, 6)	- 13(9, 5)	143812.8114(1.0)	143812.8232(0.0047)	-0.0118	160.470	155.673	
14(10, 4)	- 13(10, 3)		143861.4828(0.0051)		189.472	184.673	
14(10, 5)	- 13(10, 4)	143861.4711(1.0)	143861.4828(0.0051)	-0.0117	189.472	184.673	
14(11, 3)	- 13(11, 2)		143917.1398(0.0059)		221.433	216.633	
14(11, 4)	- 13(11, 3)	143917.1409(1.0)	143917.1398(0.0059)	0.0011	221.433	216.633	
14(12, 2)	- 13(12, 1)		143979.4293(0.0079)		256.327	251.525	
14(12, 3)	- 13(12, 2)	143979.4345(1.0)	143979.4293(0.0079)	0.0052	256.327	251.525	
14(13, 1)	- 13(13, 0)		144048.1413(0.0118)		294.125	289.320	
14(13, 2)	- 13(13, 1)	144048.1496(1.0)	144048.1413(0.0118)	0.0083	294.125	289.320	
15(0,15)	- 14(0,14)	151565.9141(1.0)	151565.9079(0.0036)	0.0062	40.718	35.662	
15(1,14)	- 14(1,13)		157010.8068(0.0038)		43.537	38.300	
15(1,15)	- 14(1,14)	149399.4894(1.0)	149399.4998(0.0035)	-0.0104	41.481	36.498	

TABLE I. OBSERVED AND CALCULATED FREQUENCIES OF VINYL ISOCYANIDE IN MHz (CONTINUED)

TRANSITION UPPER STATE	TRANSITION LOWER STATE	OBSERVED FREQUENCY (WEIGHT)	CALCULATED FREQUENCY (STANDARD DEVIATION)	OBS.-CALC.	ENERGY LEVELS IN CM-1 UPPER STATE	ENERGY LEVELS IN CM-1 LOWER STATE	REMARKS
15(2,13)	14(2,12)		155657.2428(0.0035)		47.506	42.314	
15(2,14)	14(2,13)	153425.7939(1.0)	153425.8113(0.0034)	-0.0174	47.179	42.061	
15(3,12)	14(3,11)	154213.5532(1.0)	154213.5388(0.0031)	0.0144	55.012	49.868	
15(3,13)	14(3,12)	154075.6701(1.0)	154075.6746(0.0031)	-0.0045	54.998	49.859	
15(4,11)	14(4,10)	154023.3872(1.0)	154023.3894(0.0029)	-0.0022	65.793	60.656	
15(4,12)	14(4,11)	154020.2789(1.0)	154020.2861(0.0029)	-0.0072	65.793	60.656	
15(5,10)	14(5, 9)	153987.7642(1.0)	153987.7995(0.0031)	-0.0353	79.665	74.528	
15(5,11)	14(5,10)	153987.7642(1.0)	153987.7641(0.0031)	0.0001	79.665	74.528	
15(6, 9)	14(6, 8)		153988.8198(0.0035)		96.600	91.464	
15(6,10)	14(6, 9)	153988.8411(1.0)	153988.8195(0.0035)	0.0216	96.600	91.464	
15(7, 8)	14(7, 7)		154008.9321(0.0041)		116.582	111.445	
15(7, 9)	14(7, 8)	154008.9169(1.0)	154008.9321(0.0041)	-0.0152	116.582	111.445	
15(8, 7)	14(8, 6)		154041.8575(0.0046)		139.592	134.454	
15(8, 8)	14(8, 7)	154041.8662(1.0)	154041.8575(0.0046)	0.0087	139.592	134.454	
15(9, 6)	14(9, 5)		154084.7283(0.0049)		165.610	160.470	
15(9, 7)	14(9, 6)	154084.7516(1.0)	154084.7283(0.0049)	0.0233	165.610	160.470	
15(10, 5)	14(10, 4)		154136.0864(0.0049)		194.613	189.472	
15(10, 6)	14(10, 5)	154136.0941(1.0)	154136.0864(0.0049)	0.0077	194.613	189.472	
15(11, 4)	14(11, 3)		154195.1357(0.0053)		226.577	221.433	
15(11, 5)	14(11, 4)	154195.1535(1.0)	154195.1357(0.0053)	0.0178	226.577	221.433	
15(12, 3)	14(12, 2)		154261.4219(0.0070)		261.473	256.327	
15(12, 4)	14(12, 3)	154261.4638(1.0)	154261.4219(0.0070)	0.0419	261.473	256.327	
15(13, 2)	14(13, 1)		154334.6797(0.0111)		299.273	294.125	
15(13, 3)	14(13, 2)	154334.6527(1.0)	154334.6797(0.0111)	-0.0270	299.273	294.125	
15(14, 1)	14(14, 0)		154414.7564(0.0174)		339.944	334.794	
15(14, 2)	14(14, 1)	154414.7077(0.0)	154414.7564(0.0174)	-0.0487	339.944	334.794	f
16(0,16)	15(0,15)		161392.9059(0.0039)		46.102	40.718	
16(1,15)	15(1,14)		167360.8434(0.0043)		49.120	43.537	
16(1,16)	15(1,15)		159287.2667(0.0038)		46.794	41.481	
16(2,14)	15(2,13)		166241.9048(0.0040)		53.052	47.506	
16(2,15)	15(2,14)		163590.8091(0.0038)		52.635	47.179	
16(3,13)	15(3,12)		164556.5640(0.0035)		60.501	55.012	
16(3,14)	15(3,13)		164366.5531(0.0036)		60.481	54.998	
16(4,12)	15(4,11)		164311.4056(0.0034)		71.274	65.793	
16(4,13)	15(4,12)		164306.5023(0.0034)		71.274	65.793	
16(5,11)	15(5,10)		164263.6546(0.0036)		85.144	79.665	
16(5,12)	15(5,11)		164263.5903(0.0036)		85.144	79.665	
16(6,10)	15(6, 9)		164260.0360(0.0041)		102.079	96.600	
16(6,11)	15(6,10)		164260.0355(0.0041)		102.079	96.600	
16(7, 9)	15(7, 8)		164278.7103(0.0048)		122.062	116.582	
16(7,10)	15(7, 9)		164278.7103(0.0048)		122.062	116.582	
16(8, 8)	15(8, 7)		164312.0398(0.0054)		145.073	139.592	
16(8, 9)	15(8, 8)		164312.0398(0.0054)		145.073	139.592	
16(9, 7)	15(9, 6)		164356.5398(0.0058)		171.092	165.610	
16(9, 8)	15(9, 7)		164356.5398(0.0058)		171.092	165.610	
16(10, 6)	15(10, 5)		164410.4362(0.0058)		200.097	194.613	
16(10, 7)	15(10, 6)		164410.4362(0.0058)		200.097	194.613	
16(11, 5)	15(11, 4)		164472.7579(0.0061)		232.063	226.577	
16(11, 6)	15(11, 5)		164472.7579(0.0061)		232.063	226.577	
16(12, 4)	15(12, 3)		164542.9475(0.0076)		266.961	261.473	
16(12, 5)	15(12, 4)		164542.9475(0.0076)		266.961	261.473	
16(13, 3)	15(13, 2)		164620.6767(0.0116)		304.764	299.273	

TABLE I. OBSERVED AND CALCULATED FREQUENCIES OF VINYL ISOCYANIDE IN MHz (CONTINUED)

TRANSITION UPPER STATE	TRANSITION LOWER STATE	OBSERVED FREQUENCY (WEIGHT)	CALCULATED FREQUENCY (STANDARD DEVIATION)	OBS.-CALC.	ENERGY LEVELS IN CM-1 UPPER STATE	ENERGY LEVELS IN CM-1 LOWER STATE	REMARKS
16(13, 4) -	15(13, 3)		164620.6767(0.0116)		304.764	299.273	
16(14, 2) -	15(14, 1)		164705.7527(0.0181)		345.438	339.944	
16(14, 3) -	15(14, 2)		164705.7527(0.0181)		345.438	339.944	
16(15, 1) -	15(15, 0)		164798.0671(0.0275)		388.951	383.454	
16(15, 2) -	15(15, 1)		164798.0671(0.0275)		388.951	383.454	
17(0,17) -	16(0,16)	171186.3604(1.0)	171186.3290(0.0044)	0.0314	51.812	46.102	
17(1,16) -	16(1,15)	177684.9716(1.0)	177685.0023(0.0049)	-0.0307	55.046	49.120	
17(1,17) -	16(1,16)	169163.8916(1.0)	169163.8933(0.0043)	-0.0017	52.437	46.794	
17(2,15) -	16(2,14)	176846.3929(1.0)	176846.3864(0.0047)	0.0065	58.951	53.052	
17(2,16) -	16(2,15)	173743.8150(1.0)	173743.8208(0.0044)	-0.0058	58.431	52.635	
17(3,14) -	16(3,13)	174914.8160(1.0)	174914.8164(0.0042)	-0.0004	66.336	60.501	
17(3,15) -	16(3,14)	174658.3503(1.0)	174658.3589(0.0042)	-0.0086	66.307	60.481	
17(4,13) -	16(4,12)	174603.5222(1.0)	174603.5246(0.0041)	-0.0024	77.098	71.274	
17(4,14) -	16(4,13)	174596.0032(1.0)	174595.9990(0.0041)	0.0042	77.098	71.274	
17(5,12) -	16(5,11)	174541.3877(0.0)	174541.4455(0.0044)	-0.0578	90.966	85.144	b
17(5,13) -	16(5,12)	174541.3877(0.0)	174541.3331(0.0044)	0.0546	90.966	85.144	b
17(6,11) -	16(6,10)		174532.2694(0.0051)		107.901	102.079	
17(6,12) -	16(6,11)	174532.2586(1.0)	174532.2684(0.0051)	-0.0098	107.901	102.079	
17(7,10) -	16(7, 9)		174548.9696(0.0060)		127.884	122.062	
17(7,11) -	16(7,10)	174548.9850(1.0)	174548.9695(0.0060)	0.0155	127.884	122.062	
17(8, 9) -	16(8, 8)		174582.3580(0.0069)		150.896	145.073	
17(8,10) -	16(8, 9)	174582.3478(1.0)	174582.3580(0.0069)	-0.0102	150.896	145.073	
17(9, 8) -	16(9, 7)		174628.2505(0.0076)		176.917	171.092	
17(9, 9) -	16(9, 8)	174628.2394(1.0)	174628.2505(0.0076)	-0.0111	176.917	171.092	
17(10, 7) -	16(10, 6)		174684.5148(0.0081)		205.924	200.097	
17(10, 8) -	16(10, 7)	174684.5393(1.0)	174684.5148(0.0081)	0.0245	205.924	200.097	
17(11, 6) -	16(11, 5)		174749.9810(0.0087)		237.892	232.063	
17(11, 7) -	16(11, 6)	174749.9975(1.0)	174749.9810(0.0087)	0.0165	237.892	232.063	
17(12, 5) -	16(12, 4)		174823.9747(0.0104)		272.793	266.961	
17(12, 6) -	16(12, 5)	174823.9681(1.0)	174823.9747(0.0104)	-0.0066	272.793	266.961	
17(13, 4) -	16(13, 3)		174906.0959(0.0141)		310.598	304.764	
17(13, 5) -	16(13, 4)	174906.0674(1.0)	174906.0959(0.0141)	-0.0285	310.598	304.764	
17(14, 3) -	16(14, 2)		174996.1060(0.0206)		351.276	345.438	
17(14, 4) -	16(14, 3)	174995.9820(0.0)	174996.1060(0.0206)	-0.1240	351.276	345.438	f
17(15, 2) -	16(15, 1)		175093.8671(0.0302)		394.791	388.951	
17(15, 3) -	16(15, 2)	175093.6643(0.0)	175093.8671(0.0302)	-0.2028	394.791	388.951	f
17(16, 1) -	16(16, 0)		175199.3069(0.0430)		441.110	435.266	
17(16, 2) -	16(16, 1)	175198.9551(0.0)	175199.3069(0.0430)	-0.3518	441.110	435.266	f
** A TYPE Q BRANCH **							
1(1, 0) -	1(1, 1)		517.5954(0.0002)		1.897	1.879	
2(1, 1) -	2(1, 2)		1552.7597(0.0005)		2.598	2.546	
3(1, 2) -	3(1, 3)		3105.4177(0.0010)		3.650	3.547	
4(1, 3) -	4(1, 4)		5175.3996(0.0017)		5.053	4.880	
5(1, 4) -	5(1, 5)		7762.3735(0.0024)		6.806	6.547	
6(1, 5) -	6(1, 6)	10865.7605(1.0)	10865.7548(0.0032)	0.0057	8.909	8.546	
7(1, 6) -	7(1, 7)	14484.5980(1.0)	14484.5939(0.0041)	0.0041	11.362	10.879	
8(1, 7) -	8(1, 8)	18617.7300(0.0)	18617.4419(0.0049)	0.2881	14.165	13.544	a
9(1, 8) -	9(1, 9)		23262.1958(0.0058)		17.317	16.541	
10(1, 9) -	10(1,10)		28415.9235(0.0066)		20.817	19.869	
11(1,10) -	11(1,11)		34074.6710(0.0074)		24.667	23.530	

TABLE I. OBSERVED AND CALCULATED FREQUENCIES OF VINYL ISOCYANIDE IN MHz (CONTINUED)

TRANSITION UPPER STATE	TRANSITION LOWER STATE	OBSERVED FREQUENCY (WEIGHT)	CALCULATED FREQUENCY (STANDARD DEVIATION)	OBS.-CALC.	ENERGY LEVELS IN CM-1 UPPER STATE	ENERGY LEVELS IN CM-1 LOWER STATE	REMARKS
8(2, 6) -	8(2, 7)		905.4963(0.0011)		18.525	18.494	
9(2, 7) -	9(2, 8)		1419.1283(0.0015)		21.618	21.571	
10(2, 8) -	10(2, 9)		2121.0821(0.0021)		25.059	24.988	
11(2, 9) -	11(2,10)		3049.5319(0.0028)		28.848	28.746	
12(2,10) -	12(2,11)		4244.1641(0.0036)		32.986	32.844	
13(2,11) -	13(2,12)		5745.2148(0.0044)		37.474	37.283	
14(2,12) -	14(2,13)		7592.4046(0.0052)		42.314	42.061	
15(2,13) -	15(2,14)	9823.8415(1.0)	9823.8361(0.0059)	0.0054	47.506	47.179	
16(2,14) -	16(2,15)	12474.9355(1.0)	12474.9318(0.0065)	0.0037	53.052	52.635	
17(2,15) -	17(2,16)	15577.4985(1.0)	15577.4974(0.0069)	0.0011	58.951	58.431	
18(2,16) -	18(2,17)		19158.9817(0.0072)		65.204	64.565	
19(2,17) -	19(2,18)		23241.9820(0.0075)		71.811	71.036	
17(3,14) -	17(3,15)		862.2259(0.0027)		66.336	66.307	
18(3,15) -	18(3,16)		1201.9480(0.0034)		72.516	72.476	
19(3,16) -	19(3,17)		1644.4243(0.0041)		79.044	78.989	
20(3,17) -	20(3,18)		2211.9187(0.0049)		85.918	85.845	
21(3,18) -	21(3,19)		2929.5024(0.0057)		93.141	93.044	
22(3,19) -	22(3,20)		3825.0012(0.0064)		100.713	100.586	
23(3,20) -	23(3,21)		4928.8390(0.0070)		108.635	108.471	
24(3,21) -	24(3,22)		6273.7603(0.0074)		116.908	116.698	
25(3,22) -	25(3,23)		7894.4224(0.0075)		125.532	125.268	
26(3,23) -	26(3,24)	9826.8490(1.0)	9826.8517(0.0074)	-0.0027	134.509	134.181	
27(3,24) -	27(3,25)	12107.7685(1.0)	12107.7705(0.0071)	-0.0020	143.839	143.435	
28(3,25) -	28(3,26)	14773.7770(1.0)	14773.8143(0.0070)	-0.0373	153.524	153.031	
29(3,26) -	29(3,27)	17860.6625(1.0)	17860.6707(0.0076)	-0.0082	163.565	162.969	
37(4,33) -	37(4,34)	8166.5600(1.0)	8166.5540(0.0079)	0.0060	266.071	265.799	
38(4,34) -	38(4,35)	9938.6360(1.0)	9938.6343(0.0075)	0.0017	279.179	278.848	
39(4,35) -	39(4,36)	12013.5010(1.0)	12013.4983(0.0079)	0.0027	292.640	292.239	
40(4,36) -	40(4,37)	14426.0005(1.0)	14425.9893(0.0097)	0.0112	306.456	305.975	
41(4,37) -	41(4,38)	17211.7235(1.0)	17211.7178(0.0128)	0.0057	320.627	320.053	
50(5,45) -	50(5,46)	8923.0175(1.0)	8923.0164(0.0130)	0.0011	476.258	475.960	
51(5,46) -	51(5,47)	10674.1060(1.0)	10674.1267(0.0120)	-0.0207	493.839	493.483	
52(5,47) -	52(5,48)	12705.6035(1.0)	12705.6025(0.0109)	0.0010	511.772	511.349	
53(5,48) -	53(5,49)	15049.7805(1.0)	15049.7884(0.0123)	-0.0079	530.060	529.558	
54(5,49) -	54(5,50)	17740.3840(1.0)	17740.3796(0.0198)	0.0044	548.703	548.112	
** B TYPE P BRANCH **							
1(1, 1) -	2(0, 2)	25582.8300(1.0)	25582.8808(0.0030)	-0.0508	1.879	1.026	a
2(1, 2) -	3(0, 3)	14827.6000(1.0)	14827.6308(0.0029)	-0.0008	2.546	2.052	
3(1, 3) -	4(0, 4)		3837.2868(0.0030)		3.547	3.419	
5(0, 5) -	4(1, 4)		7373.9889(0.0032)		5.126	4.880	
6(0, 6) -	5(1, 5)	18788.9200(0.0)	18788.8265(0.0035)	0.0935	7.174	6.547	a
7(0, 7) -	6(1, 6)	30386.7500(1.0)	30386.7404(0.0037)	0.0096	9.560	8.546	a
8(0, 8) -	7(1, 7)		42144.3016(0.0040)		12.285	10.879	
9(0, 9) -	8(1, 8)		54035.4165(0.0043)		15.346	13.544	
10(0,10) -	9(1, 9)		66031.7383(0.0045)		18.743	16.541	
11(0,11) -	10(1,10)		78103.2275(0.0047)		22.475	19.869	
12(0,12) -	11(1,11)	90218.8987(1.0)	90218.8634(0.0048)	0.0353	26.539	23.530	
9(2, 8) -	10(1, 9)		22584.5447(0.0078)		21.571	20.817	

TABLE I. OBSERVED AND CALCULATED FREQUENCIES OF VINYL ISOCYANIDE IN MHz (CONTINUED)

TRANSITION UPPER STATE	TRANSITION LOWER STATE	OBSERVED FREQUENCY (WEIGHT)	CALCULATED FREQUENCY (STANDARD DEVIATION)	OBS.-CALC.	ENERGY LEVELS IN CM-1 UPPER STATE	ENERGY LEVELS IN CM-1 LOWER STATE	REMARKS
10(2, 9) -	11(1,10)	9631.6150(1.0)	9631.6199(0.0079)	-0.0049	24.988	24.667	
12(1,11) -	11(2,10)		3537.5903(0.0080)		28.864	28.746	
13(1,12) -	12(2,11)	16914.5055(1.0)	16914.5056(0.0081)	-0.0001	33.408	32.844	
14(1,13) -	13(2,12)		30489.2652(0.0083)		38.300	37.283	
15(1,14) -	14(2,13)		44250.5853(0.0085)		43.537	42.061	
20(1,19) -	19(2,18)	115343.9007(1.0)	115343.9237(0.0123)	-0.0230	74.884	71.036	
17(2,15) -	18(1,18)	16239.7515(1.0)	16239.7453(0.0096)	0.0062	58.951	58.409	
18(2,16) -	19(1,19)	14821.3660(1.0)	14821.3522(0.0096)	0.0138	65.204	64.709	
19(2,17) -	20(1,20)	14187.6745(1.0)	14187.6861(0.0096)	-0.0116	71.811	71.338	
20(2,18) -	21(1,21)	14352.8510(1.0)	14352.8515(0.0098)	-0.0005	78.774	78.295	
21(2,19) -	22(1,22)		15324.9941(0.0112)		86.091	85.580	
22(2,20) -	23(1,23)	17106.5060(1.0)	17106.5116(0.0148)	-0.0056	93.762	93.192	
23(2,21) -	24(1,24)		19694.4190(0.0218)		101.787	101.130	
13(3,10) -	14(2,13)	90173.8409(1.0)	90173.8124(0.0142)	0.0285	45.069	42.061	
22(3,19) -	23(2,22)	12663.3145(1.0)	12663.3183(0.0071)	-0.0038	100.713	100.291	
23(3,20) -	24(2,23)		5720.4746(0.0070)		108.635	108.444	
25(2,24) -	24(3,21)		744.2987(0.0075)		116.932	116.908	
26(2,25) -	25(3,22)		6686.7179(0.0086)		125.755	125.532	
27(2,27) -	26(3,23)	12062.0525(1.0)	12062.0446(0.0106)	0.0079	134.911	134.509	
28(2,27) -	27(3,24)	16825.8260(1.0)	16825.8256(0.0135)	0.0004	144.401	143.839	
28(4,25) -	29(3,26)	8410.3950(1.0)	8410.3988(0.0144)	-0.0038	163.845	163.565	
30(4,26) -	31(3,29)	8427.5350(1.0)	8427.5456(0.0113)	-0.0106	184.147	183.866	
29(4,25) -	30(3,28)	17742.8355(1.0)	17742.8439(0.0119)	-0.0084	173.839	173.247	
33(3,31) -	32(4,28)	9497.7605(1.0)	9497.7724(0.0127)	-0.0119	206.123	205.807	
37(5,33) -	38(4,34)	10488.2445(1.0)	10488.2481(0.0188)	-0.0036	279.529	279.179	
40(4,36) -	39(5,35)	14971.8055(1.0)	14971.7990(0.0144)	0.0065	306.456	305.956	
38(5,33) -	39(4,36)	10591.0740(1.0)	10591.0624(0.0148)	0.0116	292.593	292.239	
41(4,38) -	40(5,35)	9847.5965(1.0)	9847.5974(0.0194)	-0.0009	320.053	319.724	
46(6,41) -	47(5,42)	11340.4120(0.0)	11340.4586(0.0334)	-0.0466	426.006	425.628	gg
49(5,44) -	48(6,43)	12788.8075(0.0)	12788.7225(0.0922)	0.0850	459.030	458.603	gg
46(6,40) -	47(5,43)	16652.6210(0.0)	16652.6580(0.0912)	-0.0370	426.015	425.459	gg
50(5,46) -	49(6,43)	15707.7480(0.0)	15707.6437(0.1003)	0.1043	475.960	475.436	gg
** B TYPE Q BRANCH **							
1(1, 0) -	1(0, 1)		46607.2404(0.0034)		1.897	0.342	
2(1, 1) -	2(0, 2)		47129.5567(0.0034)		2.598	1.026	
3(1, 2) -	3(0, 3)		47921.1119(0.0034)		3.650	2.052	
4(1, 3) -	4(0, 4)		48991.5567(0.0034)		5.053	3.419	
5(1, 4) -	5(0, 5)		50353.6618(0.0035)		6.806	5.126	
6(1, 5) -	6(0, 6)		52023.1992(0.0037)		8.909	7.174	
7(1, 6) -	7(0, 7)		54018.7477(0.0039)		11.362	9.560	
8(1, 7) -	8(0, 8)		56361.3971(0.0042)		14.165	12.285	
9(1, 8) -	9(0, 9)		59074.3234(0.0045)		17.317	15.346	

TABLE I. OBSERVED AND CALCULATED FREQUENCIES OF VINYL ISOCYANIDE IN MHz (CONTINUED)

TRANSITION UPPER STATE	TRANSITION LOWER STATE	OBSERVED FREQUENCY (WEIGHT)	CALCULATED FREQUENCY (STANDARD DEVIATION)	OBS.-CALC.	ENERGY LEVELS IN CM-1 UPPER STATE	ENERGY LEVELS IN CM-1 LOWER STATE	REMARKS
10(1, 9) -	10(0,10)		62182.2114(0.0049)		20.817	18.743	
11(1,10) -	11(0,11)		65710.5079(0.0053)		24.667	22.475	
12(1,11) -	12(0,12)	69684.5272(1.0)	69684.5079(0.0058)	0.0193	28.864	26.539	
16(1,15) -	16(0,16)	90476.4064(1.0)	90476.4055(0.0080)	0.0009	49.120	46.102	
23(1,22) -	23(0,23)	146689.7152(1.0)	146689.7083(0.0168)	0.0069	97.781	92.888	
11(2, 9) -	11(1,10)	125340.6227(1.0)	125340.6419(0.0069)	-0.0192	28.848	24.667	
12(2,10) -	12(1,11)	123572.1772(1.0)	123572.1865(0.0068)	-0.0093	32.986	28.864	
13(2,11) -	13(1,12)	121893.2605(1.0)	121893.2280(0.0067)	0.0325	37.474	33.408	
14(2,12) -	14(1,13)	120352.6338(1.0)	120352.6261(0.0066)	0.0077	42.314	38.300	
15(2,13) -	15(1,14)	118999.0645(1.0)	118999.0621(0.0066)	0.0024	47.506	43.537	
16(2,14) -	16(1,15)	117880.1204(1.0)	117880.1234(0.0066)	-0.0030	53.052	49.120	
17(2,15) -	17(1,16)	117041.0589(0.0)	117041.5074(0.0066)	-0.4485	58.951	55.046	e
18(2,16) -	18(1,17)	116526.3400(1.0)	116526.4086(0.0065)	-0.0686	65.204	61.317	
19(2,17) -	19(1,18)	116375.1730(1.0)	116375.1264(0.0064)	0.0466	71.811	67.930	
20(2,18) -	20(1,19)	116624.9257(1.0)	116624.8984(0.0062)	0.0273	78.774	74.884	
21(2,19) -	21(1,20)	117309.8798(1.0)	117309.9245(0.0060)	-0.0447	86.091	82.178	
22(2,20) -	22(1,21)	118461.5336(1.0)	118461.5235(0.0063)	0.0101	93.762	89.811	
23(2,21) -	23(1,22)	120108.3397(1.0)	120108.3420(0.0073)	-0.0023	101.787	97.781	
24(2,22) -	24(1,23)	122276.5537(1.0)	122276.5379(0.0091)	0.0158	110.166	106.087	
25(2,23) -	25(1,24)	124989.8609(1.0)	124989.8657(0.0116)	-0.0048	118.898	114.728	
** B TYPE R BRANCH **							
8(1, 8) -	7(0, 7)	119422.4179(1.0)	119422.4107(0.0059)	0.0072	13.544	9.560	

a) Reported in Ref.(5).
b) Unresolved K-doublet.
c) Several lines are overlapping.
d) Partially resolved K-doublet.
e) Not used in the fit: poor measurement.
f) Not used in the fit: Higher order centrifugal distortion correction might be necessary.
g) Not used in the fit.

Table II. Spectral parameters of vinyl isocyanide for Watson's reduced Hamiltonian in I^r axis presentation.

$\tilde{A}$	51479.4578(30) [a]	MHz
$\tilde{B}$	5386.64856(25)	MHz
$\tilde{C}$	4868.94021(25)	MHz
Δ_J	2.47615(63)	kHz
Δ_{JK}	−100.0082(69)	kHz
Δ_K	3421.08(40)	kHz
δ_J	0.549200(89)	kHz
δ_K	27.203(20)	kHz
H_J	0.00860(55)	Hz
H_{JK}	−0.444(68)	Hz
H_{KJ}	4.08(22)	Hz
H_K	328.6(118)	Hz
h_J	0.00329(23)	Hz
h_{JK}	0.326(98)	Hz
h_K	50.6(75)	Hz

$\varkappa = -0.977786$ $\quad b_p = -5.58457 \times 10^{-3}$

[a] The standard deviation of the fit is 19.5 kHz for 173 equally weighted lines. Numbers in parentheses are standard errors.

Table III. Watson's determinable rotational constants and quartic centrifugal distortion constants [a] for vinyl isocyanide.

$\mathfrak{A}$	51479.4628(30)	MHz
$\mathfrak{B}$	5386.49800(25)	MHz
$\mathfrak{C}$	4868.90066(25)	MHz
$\tau'_{aaaa} = \hbar^4 \tau_{aaaa}$	−13.2942(16)	MHz
$\tau'_{bbbb} = \hbar^4 \tau_{bbbb}$	$-14.2982(26) \times 10^{-3}$	MHz
$\tau'_{cccc} = \hbar^4 \tau_{cccc}$	$-5.5110(26) \times 10^{-3}$	MHz
τ_1	0.370319(29)	MHz
$\tau_2/(\mathfrak{A}+\mathfrak{B}+\mathfrak{C})$	$24.2529(35) \times 10^{-3}$	MHz
$\Delta\tau'_{cccc}$ [b]	$-0.1334(11) \times 10^{-3}$	MHz

[a] Numbers in the parentheses are estimated errors on the basis of the standard error of spectral constants in Table II.

[b] τ-defect: $\Delta\tau'_{cccc} = \tau'_{cccc} - (\tau_2 - \mathfrak{C}\,\tau_1)/(\mathfrak{A}+\mathfrak{B})$.

we can determine the four constants, τ_{aabb}, τ_{bbcc}, τ_{ccaa}, and τ_{abab}, which do not vanish for a planar molecule. Since the τ-defect does not vanish in the present case, different values are obtained for these four constants depending on the way the planarity conditions are used as pointed out by Kirchhoff [15] and Cook et alias [16, 17]. However, the specific equations used have not been explicitly stated by these authors. In order to show the differences among the various methods clearly, the methods used in the present analysis are compared here. The constants in the first column of Table IV are obtained by the use of Eqs. (3), (4), and (5), and the observed τ_1. Those in the second column are obtained by the use of Eqs. (3), (4), and (5), and the observed τ_2. Those in the third column are obtained by the use of Eqs. (3) and (4), and the observed τ_1 and τ_2. Those in the fourth column are obtained by the use of Eqs. (3) and (5), and the observed τ_1 and τ_2. Those in the last column are obtained from the observed τ_1 and τ_2, and the two linear combinations of the three equations, (3), (4), and (5),

$$\tau_{aacc} = (C^2/A^2)\,\tau_{aaaa} + (C^2/B^2)\,\tau_{aabb}, \tag{6}$$

$$\tau_{bbcc} = (C^2/A^2)\,\tau_{aabb} + (C^2/B^2)\,\tau_{bbbb}, \tag{7}$$

which are linearly independent with

$$\Delta\tau'_{cccc} = 0 \tag{8}$$

relating the observed τ_1, τ_2, and τ'_{cccc}. The obtained variations of the constants are not large for the V − NC molecule, but considerably larger than the estimated errors originating from the standard errors of the spectroscopic constants listed in Table II. Since we have no means to eliminate the vibrational effect from these constants, the obtained constants for the various methods are listed parallel with each other. The differences between the constants obtained from the different methods exemplify the fact that such variations are proportional to τ-defect as discussed by the present authors [18].

It should be noted that we used the determinable rotational constants, $\mathfrak{A}$, $\mathfrak{B}$, and $\mathfrak{C}$, for the ground vibrational state obtained in the present study in the planarity conditions, Eqs. (3) – (7), instead of the equilibrium rotational constants.

Excluding all contributions of centrifugal distortion from the determinable rotational constants, the effective rotational constants in the ground state, which are represented as α', β', and γ' of Kivelson und Wilson [7], are obtained as listed in Table IV. The effective moments of inertia and the inertia defect determined from these constants are also listed in Table IV.

b) Validity of the Reduced Hamiltonian and Choice of Axis Representation

From the infinite number of unitary transformations which can be applied to the effective rotational Hamiltonian we want to choose an appropriate one, by which we mean one which reduces the number of spectral constants to the number of determinable parameters following Watson's discussion [6]. Next, we have to check that the transformation does not generate unignorable higher order terms with contributions above up to sextic terms, because we hope to truncate the Hamiltonian as in Equation (1). This

check can be done by numerically evaluating s_{111}, which is the coefficient of the unitary transformation, as discussed by Watson [6]. Such a check was carried out for various molecules by Carpenter [19] and Creswell and Mills [20].

The unitary transformation used in the present analysis is the one originally proposed by Watson [6] which reduces R_6 to zero and gives the Hamiltonian shown in Equation (1). The s_{111} for this transformation can be calculated on the basis of the τ's by the use of

$$s_{111} = 4\,R_6/(X-Y) \tag{9}$$

where $$R_6 = (\tau'_{xxxx} + \tau'_{yyyy} - 2\,\tau'_{xxyy})/64\,. \tag{10}$$

Rewriting Eqs. (9) and (10) in the I^r axis representation, which has been used in the present analysis, the s_{111} coefficient was obtained for the unitary transformation used in the present analysis for each set of τ's as listed in Table IV, and they are reasonably small indicating the validity of the reduction. The I^r axis representation is the best choice of axis system for the present molecule, V – NC, a near prolate top, if only the rigid rotor Hamiltonian is considered. In the reduction of the effective rotational Hamiltonian, however, the I^r representation is not always the best choice of axis system [19, 20]. We therefore checked the other choices of the axis representation by the evaluation of s_{111}. If the III^r axis representation is used, the denominator in Eq. (9) has the largest value and a small s_{111} seems to be expected. However, for the unitary transformation which reduces $R_6 = 0$ in the III^r axis representation, the order of magnitude of s_{111} is 10^{-5}, which is considerably larger than the upper limit of s_{111} for convergence of the power series expansion of the reduced Hamiltonian. Almost the same result is obtained in the II^r axis representation.

The reduction which makes $R_5 = 0$ instead of $R_6 = 0$ is one of the other possibilities of the reduction process [21, 22]. For this reduction s_{111} is expressed as

$$s_{111} = 2\,R_5/(2\,Z-X-Y) \tag{11}$$

where

$$R_5 = -(\tau'_{xxxx} - \tau'_{yyyy} - 2\,\tau'_{zzxx} + 2\,\tau'_{yyzz})/32 \tag{12}$$

and is calculated to be of the order 10^{-7} for the present molecule in the I^r axis representation. This value is the same order of magnitude as that of the unitary transformation used in the present analysis. Since the reduction giving $R_6 = 0$ is computationally simpler, we conclude that the present choice of the unitary transformation is the best among those considered above.

c) *Hyperfine Structures*

No nuclear quadrupole hyperfine structure could be observed, although the lines are fairly broad at low sample pressure. The full width at half maximum of the line $1_{01} \leftarrow 0_{00}$ is 0.35 MHz at a sample pressure of 2.5×10^{-3} torr. Bolton et al. [5] also reported that no hyperfine structure was observed. In general the nuclear quadrupole hyperfine splitting caused by

Table IV. Constants derived from planarity conditions [a].

Constant	Case 1 [b]	Case 2 [c]	Case 3 [d]	Case 4 [e]	Case 5 [f]	
$\hbar^4\,\tau_{aabb}$	0.34875 (10)	0.34875 (10)	0.34875 (10)	0.34875 (10)	0.35753 (4)	MHz
$\hbar^4\,\tau_{bbcc}$	−8.563 (3)	−8.563 (3)	−8.563 (3)	−8.404 (2)	−8.484 (2)	kHz
$\hbar^4\,\tau_{ccaa}$	0.16603 (8)	0.16603 (8)	0.18028 (8)	0.16603 (8)	0.17320 (5)	MHz
$\hbar^4\,\tau_{abab}$	−67.95 (10)	−67.19 (10)	−75.07 (6)	−68.03 (9)	−75.97 (4)	kHz
α'	51479.4585 (30)	51479.4585 (30)	51479.4585 (30)	51479.4586 (30)	51479.4585 (30)	MHz
β'	5386.58101 (25)	5386.58101 (25)	5386.58814 (25)	5386.58101 (25)	5386.58460 (25)	MHz
γ'	4869.00709 (25)	4869.00784 (25)	4868.99996 (25)	4869.00701 (25)	4869.00346 (25)	MHz
I_a [g]	9.81704	9.81704	9.81704	9.81704	9.81704	amuA^2
I_b [g]	93.8213	93.7213	93.8212	93.8213	93.8212	amuA^2
I_c [g]	103.7945	103.7945	103.7946	103.7945	103.7945	amuA^2
Δ	0.156132 (7)	0.156116 (7)	0.156408 (7)	0.156134 (7)	0.156272 (7)	amuA^2
$R_6 \times 10^6$	−41.9	−41.9	−41.9	−46.9	−44.4	MHz
$S_{111} \times 10^6$	0.324	0.324	0.324	0.362	0.343	

[a] Numbers in the parentheses are estimated errors on the basis of the standard error of the spectral constants in Table II. In the case the error is not indicated the error is smaller than the last digit.

[b–f] See text.

[g] The errors of the moment of inertia are limited by the uncertainty of the conversion factor, which was taken to be I (amuA^2) = 5105376 × 10^5/B (MHz).

the nitrogen atom in the isocyanide group is much smaller than that in the cyanides. For example, the value χ_{aa} for methyl cyanide is -4.35 MHz [23] and for methyl isocyanide $+0.4885$ MHz [24]. For ethyl cyanide it is -3.3 MHz [25] and for ethyl isocyanide the hyperfine splitting has not been observed. Therefore, though the absolute value of χ_{aa} is large in vinyl cyanide, -4.21 MHz [2], it is probably much smaller for vinyl isocyanide. From the absorption profile of the $1_{01} \leftarrow 0_{00}$ transitions we can estimate the upper limit of the absolute value of χ_{aa} for vinyl isocyanide to be 0.5 MHz. Since we could not find any hint of hyperfine structure in either $^{q}Q_K$ transitions or in *b*-type transitions, it can be concluded that the absolute value of $\chi_{bb}-\chi_{cc}$ is small. The absorption profile of the $1_{01}-0_{00}$ transition of V – NC is illustrated in Fig. 6 together with that of vinyl cyanide for comparison. The hyperfine structure of V – NC estimated on the assumption $\chi_{aa}=+0.5$ MHz and $\chi_{bb}-\chi_{cc}=0.0$ MHz is indicated in the figure.

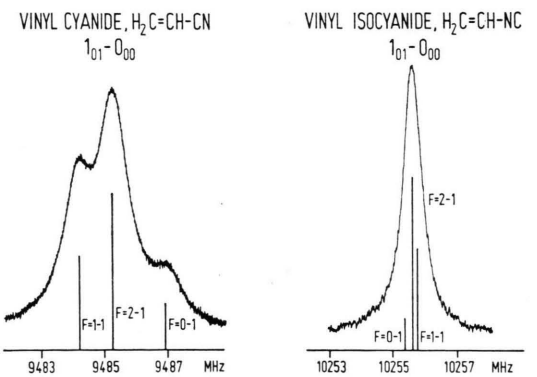

Fig. 6. The absorption profile of the a-type $1_{0,1} \leftarrow 0_{0,0}$ transition of vinyl isocyanide is compared with that of vinyl cyanide. The hyperfine structures are indicated by the line patterns showing the relative intensities. Those for vinyl isocyanide were obtained assuming $\chi_{aa}=0.05$ MHz and $\chi_{bb}-\chi_{cc}=0.0$ MHz.

d) Predicitions of line positions

Transitions of interest from a radio-astronomical point of view have been predicted and included in Table I. Figure 7 shows a part of the rotational energy level scheme of vinyl cyanide and vinyl isocyanide showing the possible transitions opportune for a radio astronomical search for this molecule. The relative magnitude of Einstein's A constant, which represents the probability of spontaneous emission, for such transitions and line strengths for all transitions listed in Table I are available from

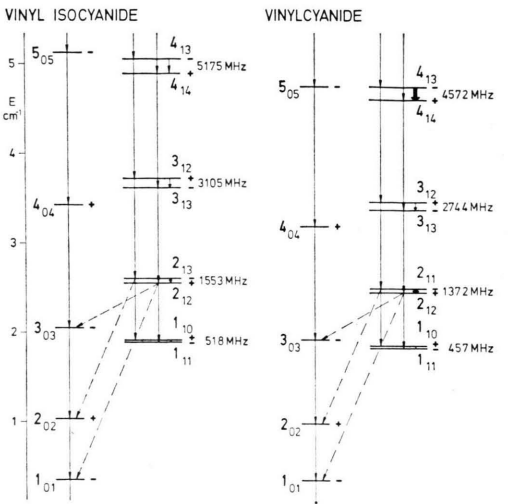

Fig. 7. Part of the rotational energy level scheme of vinyl isocyanide in the ground vibrational state as compared with that of vinyl cyanide. The solid and dashed arrows indicate **a**-type and **b**-type transitions respectively. The two heavy arrows in the diagram for vinyl cyanide indicate two **a**-type Q-branch transitions observed in Sgr B2.

the authors on request. The energy levels related to the transitions listed in Table I are also shown in the same table in cm^{-1} unit.

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