

Millimeter-wave spectroscopy of HC₅N in vibrationally excited states below 500 cm⁻¹★

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Abstract. The rotational spectrum of the semistable HC₅N molecule has been investigated in the millimeter-wave region for eight excited bending states which lie below 500 cm⁻¹, namely $v_{11} = 1, 2, 3,$ and $4, v_{10} = 1, v_9 = 1, (v_{10} = 1, v_{11} = 1),$ and $(v_{10} = 1, v_{11} = 2)$. Transitions up to $J = 101 \leftarrow 100$ were measured, reaching a frequency as high as 270 GHz. The set of spectroscopic constants determined in the present work makes it possible to predict with much improved accuracy the transition frequencies of millimeter-wave lines produced by vibrationally excited HC₅N in hot core molecular sources and circumstellar shells. In addition, results of extensive CCSD(T) calculations are presented, which yield accurate term values for low-lying bending vibrational states.

Key words. molecular data – methods: laboratory – techniques: spectroscopic – radio lines: ISM

1. Introduction

The first laboratory study of the rotational spectrum of cyanobutadiyne (HC₅N) was published by Alexander et al. (1976), who recorded the ground-state spectra of the main isotopomer and of all the mono-substituted isotopic species in the centimeter-wave (cm-wave) region, from 26 to 40 GHz. In the same year Avery et al. (1976) reported the first interstellar detection of this carbon chain in the molecular cloud Sgr B2, where the 10.65 GHz line was observed. Since that time, the number of new HC₅N sources and interstellar transitions has increased regularly, leading to the detection of emission lines also in the millimeter-wave (mm-wave) region (Winnewisser & Walmsley 1979), for the deuterated species (MacLeod et al. 1981), and for the ¹³C-containing isotopomers (Takano et al. 1990). The study of the ground-state rotational spectrum of HC₅N was extended to the mm-wave region by Winnewisser et al. (1982), and then to the submm-wave region by Bizzocchi et al. (2004). The latter paper also includes accurate

mm-wave transition frequencies for the spectra of the ¹³C and ¹⁵N-containing species of both normal and deuterated variants of cyanobutadiyne.

HC₅N has several low-lying bending vibrational states, as was theoretically predicted by Botschwina et al. (1997) through CCSD(T) calculations with the cc-pVTZ basis set. Its room-temperature rotational spectrum therefore exhibits a rich pattern of vibrational satellites, which were first analyzed by Hutchinson et al. (1980) in the 26–40 GHz region. Usually interstellar clouds are very cold, so that rotational lines from vibrationally excited states are less frequently observed by radioastronomy, although some hot core sources exhibit emissions due to rotational transitions produced by vibrationally excited molecules. For example, rotational transitions belonging to eleven vibrationally excited states of HC₃N were detected toward the hot core associated with the UC H II region G10.47+0.03 (Wyrowski et al. 1999), thus providing valuable information about the IR field which populates the vibrational levels.

More recently, mm-wave lines of vibrationally excited HC₅N were observed toward the proto-planetary nebula CRL 618 (Cernicharo et al. 2001; Thorwirth 2001; Wyrowski et al. 2003), whose thick and dusty molecular envelope is particularly rich in small hydrocarbons, which produce a rather congested mm-wave spectrum. These recent observations stimulated the present laboratory work, whose objective is a detailed analysis of the mm-wave spectra for the low-lying

★ Tables from 5 to 12 are only available in electronic form at the CDS via anonymous ftp to [cdsarc.u-strasbg.fr](ftp://cdsarc.u-strasbg.fr) (130.79.128.5) or via

<http://cdsweb.u-strasbg.fr/cgi-bin/qcat?J/A+A/425/767>

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Table 1. Calculated^a spectroscopic constants for the low-lying $v_9 = 1$, $v_{10} = 1$, and $v_{11} = 1$ singly excited bending states of HC₅N.

	$v_{11} = 1$	$v_{10} = 1$	$v_9 = 1$
ω (cm ⁻¹)	106.8	254.0	462.9
α (MHz)	-2.705	-2.453	-1.594
q_t (MHz)	1.125	0.490	0.320
$q_{t,j}$ (Hz)	-0.993	-0.176	-0.032

^a CCSD(T)/cc-pVQZ. Standard 2nd order perturbation theory in normal coordinate space is employed in the calculation of α , q_t and $q_{t,j}$ values.

excited states of HC₅N, to provide accurate rest frequencies useful for a certain identification of the corresponding radioastronomical lines. The present paper reports new mm-wave laboratory measurements for eight vibrationally excited states of cyanobutadiyne which lie below 500 cm⁻¹. The measurements were performed in the frequency range from 60 to 270 GHz and they provide very accurate values of the spectroscopic constants needed to predict precise mm-wave rest frequencies for all the excited states investigated, which are the most likely to be observable in hot molecular sources. In addition, results of more extensive CCSD(T) calculations will be presented which yield improved term values for bending vibrational states as well as a number of spectroscopic constants.

2. Results of coupled cluster calculations

The coupled cluster variant CCSD(T) (Raghavachari et al. 1989) has been employed in the calculation of a complete cubic force field for HC₅N. The cc-pVQZ basis set (Dunning Jr. 1989) was used and valence electrons were correlated in the coupled cluster calculations. These were carried out with the MOLPRO2000 suite of programs (Werner & Knowles 2000). Quantities of interest for the present paper are the energies of bending vibrational states below 500 cm⁻¹, vibration-rotation coupling constants (α) and l -type doubling constants (q_t and $q_{t,j}$). The results of the calculations are listed in Table 1. The first line contains the harmonic vibrational wavenumbers ω_{11} , ω_{10} and ω_9 which, on the basis of previous experience with calculations of this sort (Botschwina 2003), should be accurate to better than 5 cm⁻¹. Anharmonicity effects are expected to be small. Comparison with experiment is currently possible only for the bending vibration with highest wavenumber which is predominantly HCC-bending in character. The ratio $\omega_7^{(\text{theor.})}/\nu_7^{(\text{exp.})}$ is 1.013, where the experimental anharmonic wavenumber is taken from an earlier FTIR work (Haas et al. 1994). We expect differences between harmonic and anharmonic values of only about 1% also for the other bending vibrations which all correspond to heavier-atom small-amplitude vibrations. The term energies (in cm⁻¹) of low-lying excited bending vibrational states with respect to the

vibrational ground state may therefore be approximated reasonably well by the formula:

$$T(v_9, v_{10}, v_{11}) \approx \sum_{i=9}^{11} v_i \omega_i. \quad (1)$$

Making use of the data from Table 1 we arrive at eight states with energies below 500 cm⁻¹. Predictions for vibration-rotation and l -type doubling constants are made in the last lines of Table 1. As will be seen below (cf. Table 2), they are in excellent agreement with the experimental values of this work.

3. Experimental details

The excited-state rotational spectra of cyanobutadiyne have been recorded in selected frequency regions using two different source-modulation mm-wave spectrometers which operate in Cologne (I. Physikalisches Institut) and Bologna (Dipartimento di Chimica ‘‘G. Ciamician’’) respectively. The spectrometer used in Cologne for the present measurements has been described earlier (Mauer et al. 1988). The radiation sources were phase-locked solid-state Gunn oscillators with subsequent harmonic generation. Using a He-cooled InSb detector, the rotational spectra of HC₅N were recorded in the frequency range from 60 to 250 GHz. Source frequency modulation was applied and the signal was demodulated at $2f$, thus obtaining the 2nd derivative of the actual spectrum profile. The sample was prepared by a *dc* discharge in a mixture of acrylonitrile (vinyl cyanide) vapor and acetylene gas. The discharge products were collected in a trap kept at -110 °C. The sample was purified by low temperature distillation and the spectra were recorded using the portion evaporating in a temperature range from -50 to -30 °C. The absorption cell was a 4.5 m long glass tube sealed by PTFE windows. The sample pressure was in the range 0.2 to 0.4 Pa and all measurements were carried out at room temperature.

A similar spectrometer has been used in Bologna to record additional HC₅N lines between 80 and 270 GHz, and a detailed description can be found in a previous paper (Bizzocchi & Degli Esposti 2001). The main difference lies in the fact that a room-temperature Schottky-barrier diode was employed to observe the lines below 190 GHz. In addition, a completely different method was used to produce HC₅N, based on gas-phase copyrolysis ($T = 1200$ °C) of pyridine and PCl₃ in a flow reactor, as already described (Bizzocchi et al. 2004). The high-temperature reactor was connected to the absorption cell of the mm-wave spectrometer, and the HC₅N spectra were recorded while the pyrolysis products were continuously pumped through the cell.

4. Observed spectra and analysis

We have investigated the mm-wave spectra of HC₅N in the $v_{11} = 1, 2, 3$, and 4 , $v_{10} = 1$, $v_9 = 1$, ($v_{10} = 1$, $v_{11} = 1$), and ($v_{10} = 1$, $v_{11} = 2$) excited states, which all lie below 500 cm⁻¹ (cf. Table 1). Earlier cm-wave frequency data were available for all the states studied (Hutchinson et al. 1980); we have extended the measurements reaching a frequency as high as

Table 2. Spectroscopic constants determined for the ground, $v_9 = 1$, $v_{10} = 1$, and $v_{11} = 1$ fundamental bending states of HC₅N. Standard errors in units of the last digit are given in parentheses for the fitted parameters.

		Ground state ^a	$v_{11} = 1$	$v_{10} = 1$	$v_9 = 1$
B	(MHz)	1331.332687(20)	1334.118237(24)	1333.784785(26)	1332.925330(20)
α	(MHz)		-2.786	-2.452	-1.593
D	(Hz)	30.1090(15)	31.6522(17)	30.7624(19)	30.4337(14)
H	(μ Hz)	1.635(29)	1.635 ^b	1.635 ^b	1.635 ^b
$d_{JL(11,11)}$	(kHz)		-3.3047 ^b		
q_t	(MHz)		1.162898(48)	0.500190(52)	0.328526(40)
q_{tJ}	(Hz)		-1.0629(34)	-0.1734(37)	-0.0393(28)
σ_{fit}	(kHz)	7.2	14.6	10.6	8.2
No. of lines		46	98	64	65
J range		9–171	8–100	10–100	10–100

^a From Bizzocchi et al. (2004).

^b Fixed in the analysis.

270 GHz. All the mentioned states involve excitation of at least one bending quantum, so that multiplets of rotational lines were always recorded for each $J + 1 \leftarrow J$ transition, owing to l -type resonance effects between the different l sublevels. The spectra were analyzed using the formalism originally developed by Yamada and coworkers (Yamada et al. 1985; Niederhoff & Yamada 1993) and employed recently to fit the excited-state rotational spectra of the carbon chain HC₅P (Bizzocchi et al. 2003).

Briefly, the ro-vibrational Hamiltonian has been first represented using the unsymmetrized basis functions $|v_9^{l_9}, v_{10}^{l_{10}}, v_{11}^{l_{11}}; J, k\rangle$, where $k = l_9 + l_{10} + l_{11}$. Adopting the simplified notation $|l_9, l_{10}, l_{11}; k\rangle$, the diagonal elements of the Hamiltonian matrix actually employed are:

$$\begin{aligned} \langle l_9, l_{10}, l_{11}; k | \hat{H} | l_9, l_{10}, l_{11}; k \rangle = & x_{L(11,11)} l_{11}^2 + x_{L(10,11)} l_{10} l_{11} \\ & + (B_v + d_{JL(11,11)} l_{11}^2 + d_{JL(10,11)} l_{10} l_{11}) [J(J+1) - k^2] \\ & - D_v [J(J+1) - k^2]^2 + H_v [J(J+1) - k^2]^3. \end{aligned} \quad (2)$$

The x_L anharmonic constants produce a small vibrational energy separation between the various l_t sublevels of a given vibrational state, while the d_{JL} constants are high-order vibration-rotation interaction parameters which are responsible for the slight l_t dependence of the B_v constants. The main off-diagonal rotational l -type doubling terms ($\Delta l_t = \pm 2$, $\Delta k = \pm 2$) have the general form:

$$\begin{aligned} \langle l_t \pm 2; k \pm 2 | \hat{H} | l_t; k \rangle = & \frac{1}{4} [q_t + q_{tJ} J(J+1)] \\ & \times \sqrt{(v_t \mp l_t)(v_t \pm l_t + 2)} \\ & \times \sqrt{[J(J+1) - k(k \pm 1)][J(J+1) - (k \pm 1)(k \pm 2)]} \end{aligned} \quad (3)$$

while the off-diagonal vibrational l -type resonance terms ($\Delta l_{10} = \pm 2$, $\Delta l_{11} = \mp 2$, $\Delta k = 0$) have the expression:

$$\begin{aligned} \langle l_{10} \pm 2, l_{11} \mp 2; k | \hat{H} | l_{10}, l_{11}; k \rangle = & \frac{1}{4} [r_{10,11} + r_{10,11,J} J(J+1)] \\ & \times \sqrt{(v_{10} \mp l_{10})(v_{10} \pm l_{10} + 2)(v_{11} \mp l_{11} + 2)(v_{11} \pm l_{11})}. \end{aligned} \quad (4)$$

The high-order off-diagonal rotational l -type resonance term ($\Delta l_{10} = \mp 2$, $\Delta l_{11} = \pm 4$, $\Delta k = \pm 2$) was also considered for analysis of the spectrum of the ($v_{10} = 1$, $v_{11} = 2$) state:

$$\begin{aligned} \langle l_{10} \mp 2, l_{11} \pm 4; k \pm 2 | \hat{H} | l_{10}, l_{11}; k \rangle = & \\ & \frac{1}{8} q_{10,11,11} \sqrt{(v_{10} \pm l_{10})(v_{10} \mp l_{10} + 2)} \\ & \times \sqrt{(v_{11} \mp l_{11})(v_{11} \pm l_{11} + 2)(v_{11} \mp l_{11} - 2)(v_{11} \pm l_{11} + 4)} \\ & \times \sqrt{[J(J+1) - k(k \pm 1)][J(J+1) - (k \pm 1)(k \pm 2)]}. \end{aligned} \quad (5)$$

The resulting energy matrix was then factorized into symmetric and antisymmetric blocks adopting Wang-type linear combinations of wavefunctions (Yamada et al. 1985). Any sublevel belonging to a given vibrational state can therefore be labelled through its k (or l_t) value and by the “+” or “-” superscripts which designate which kind of symmetrized linear combination of wavefunctions has been chosen. Some details dealing with the analyses performed for the various vibrational states investigated are given in the following subsections. Over 650 new transition frequencies have been measured, and the complete list of analyzed data is available in electronic form at the CDS. The few cm-wave transition frequencies previously published for all of the states investigated (Hutchinson et al. 1980) have been included in the present analyses using the same weighting factor employed for the more recent mm-wave measurements.

4.1. The fundamental bending states $v_9 = 1$, $v_{10} = 1$, and $v_{11} = 1$

The measurements for the bending states $v_9 = 1$, $v_{10} = 1$ and $v_{11} = 1$ have been extended up to 270 GHz, reaching a J value as high as 100. For these states each rotational transition is split into two components because of l -type doubling. The low-frequency components of the doublets for the $v_{11} = 1$ and $v_{10} = 1$ states are accidentally superimposed up to 100 GHz, but at higher frequencies they are well separated, as Fig. 1 shows. Owing to this, the absorption frequencies measured for

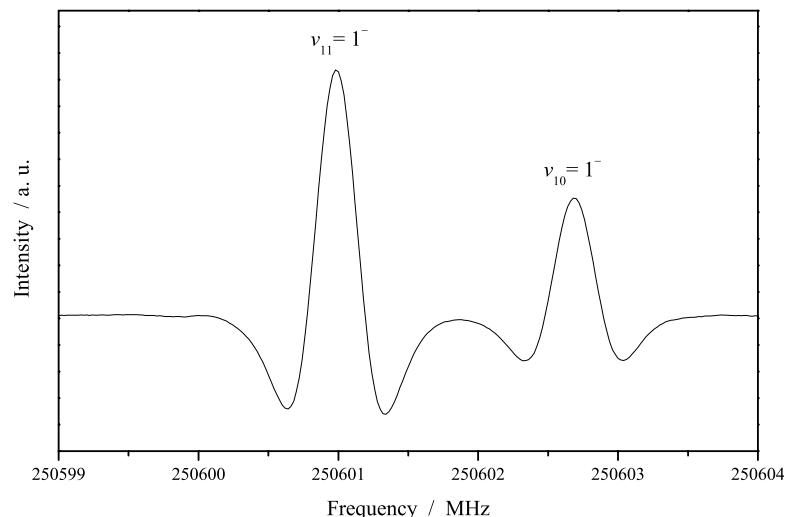


Fig. 1. Spectrum of the low frequency components for the $J = 94 \leftarrow 93$ rotational transition of HC₅N in the vibrationally excited states $v_{11} = 1$ and $v_{10} = 1$. Two scans were coadded with a total recording time of 76 s.

blended transitions were always assigned to the most populated $v_{11} = 1$ state, but they were analyzed using a six times smaller weighting factor ($w_i = 1/\sigma_i^2$). The peak-intensities observed for the excited-state lines are consistent with the theoretical values of the vibrational harmonic wavenumbers reported in Table 1. The measured frequencies have been analyzed through Eqs. (2) and (3) (having $k = l_9$, or l_{10} , or l_{11}), fitting the rotational constant B , the quartic centrifugal distortion constant D and the l -type doubling parameters q_l and $q_{l,J}$. The sextic centrifugal distortion constant H gives a small, but not completely negligible contribution to the observed frequencies, and it was therefore held fixed at the value determined for the ground state (Bizzocchi et al. 2004). This produced a decrease in the standard deviation of the fits of ca. 2 kHz. The same procedure was followed for the subsequent least-squares analyses. The lists of the experimental transition frequencies are collected in Tables 5–7; which are available in electronic form at the CDS. The results of the least squares fits are listed in Table 2, where the ground-state constants previously determined (Bizzocchi et al. 2004) and the derived vibration-rotation interaction constants (α) are also reported.

4.2. The overtone bending states $v_{11} = 2, 3$, and 4

We have extended the measurements for these overtone bending states up to 230 GHz, reaching J values as high as 85, thus making possible a more accurate analysis of the l -type resonance effects between the various l -sublevels produced by progressive excitation of the lowest energy bending mode. The high- J transitions recorded allowed us to observe l -type splittings also for the lines of the $|l_{11}| = 3$ and $|l_{11}| = 4$ sublevels, starting from the $J = 29 \leftarrow 28$ and $J = 54 \leftarrow 53$ transitions, respectively. The spectra have been analyzed using Eqs. (2) and (3), having $k = l_{11}$. The constants q_{11} and $q_{11,J}$ were fitted for the $v_{11} = 3$ state, which has degenerate $l_{11} = \pm 1$ sublevels, but they were constrained to interpolated or extrapolated values for the $v_{11} = 2$ and $v_{11} = 4$ states, respectively.

The measured transition frequencies analyzed for these overtone bending states are listed in Tables 8–10 available at the CDS, while the results of the least-squares fits are collected in Table 3.

4.3. The bending combination states ($v_{10} = 1$, $v_{11} = 1$) and ($v_{10} = 1$, $v_{11} = 2$)

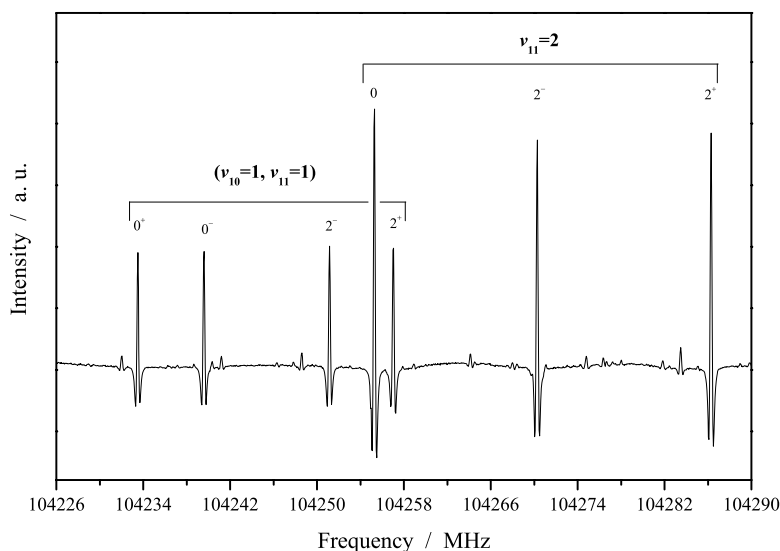
When the bending modes v_{10} and v_{11} are simultaneously excited, with $v_{10} = v_{11} = 1$, then four independent symmetrized basis functions can be built up, two of which have $k = 0$, and two $k = 2$. The resulting four sublevels can therefore be labelled as 0^+ , 0^- , 2^+ , and 2^- , and a quadruplet of lines must be expected for each $J + 1 \leftarrow J$ transition. The $J = 39 \leftarrow 38$ quadruplet of the ($v_{10} = 1$, $v_{11} = 1$) state is shown in Fig. 2, together with the nearby triplet of lines produced by the $v_{11} = 2$ state. For the bending combination in which $v_{10} = 1$ and $v_{11} = 2$, six independent symmetrized basis functions can be built up, and the corresponding substates can be indicated as -1^+ , -1^- , 1^+ , 1^- , 3^+ , and 3^- , from which six lines originate for each $J + 1 \leftarrow J$ transition. Transition frequencies have been measured up to 230 GHz, and analyzed through Eqs. (2)–(5) taking into account both rotational and vibrational l -type resonances. The q_l constants involved in the off-diagonal matrix elements were left free in both fits to obtain a better agreement between experimental and calculated frequencies. The fitted values are only slightly different from those of the corresponding fundamental bending states, as expected for a normal vibrational dependence of the q_l constants. The experimental transition frequencies are listed in Tables 11 and 12 available at the CDS. The results of the least-squares fits are collected in Table 4.

5. Conclusion

This paper extends to the mm-wave region the study of the rotational spectra for eight vibrationally excited states of HC₅N which lie below 500 cm⁻¹. All the states investigated involve

Table 3. Spectroscopic constants determined for the $v_{11} = 2, 3,$ and 4 overtone bending states of HC₅N. Standard errors in units of the last digit are given in parentheses for the fitted parameters.

		$v_{11} = 2$	$v_{11} = 3$	$v_{11} = 4$
B	(MHz)	1336.911999(30)	1339.713811(29)	1342.523686(28)
D	(Hz)	33.2316(22)	34.8337(22)	36.4611(27)
H	(μ Hz)	1.635 ^a	1.635 ^a	1.635 ^a
$d_{JL(11,11)}$	(kHz)	-3.3316(86)	-3.3585(43)	-3.3630(21)
q_l	(MHz)	1.167820 ^a	1.172741(28)	1.177662 ^a
q_{lJ}	(Hz)	-1.0779 ^a	-1.0928(30)	-1.1077 ^a
$x_{L(11,11)}$	(GHz)	6.29229(22)	6.27067(27)	6.25081(16)
σ_{fit}	(kHz)	8.9	10.1	12.8
No. of lines		85	109	115
J range		9–85	10–85	13–85

^a Fixed in the analysis.**Fig. 2.** Spectrum of the $J = 39 \leftarrow 38$ rotational transition of HC₅N for the vibrationally excited states ($v_{10} = 1, v_{11} = 1$) and $v_{11} = 2$. The total recording time was 195 s.

excitation of at least one bending quantum, so that l -type resonance effects had to be taken into account in the analysis of the spectra to obtain spectroscopic parameters with a clear physical meaning. At present, this paper provides the best set of rest frequencies for rotational transitions of the low-lying vibrational excited states of HC₅N, whose mm-wave lines have recently been detected in CRL 618 (Cernicharo et al. 2001; Thorwirth 2001; Wyrowski et al. 2003). The improved set of spectroscopic constants derived from the analysis of the spectra makes it possible now to predict excited-state line frequencies with uncertainties of a few kHz at $\lambda = 2$ mm (1σ level). In comparison with previous results (Hutchinson et al. 1980), the accuracy of the predicted frequencies has been improved by more than two orders of magnitude, thus making possible more reliable assignments of radio lines due to the rather dense spectrum produced by vibrationally excited HC₅N. As an example, it can be mentioned that a feature observed at 101.74 GHz in the radio spectrum of CRL 618 (Cernicharo et al. 2001, Fig. 3) has been assigned to the unresolved $|l_{10}| = 3$ doublet of the

$v_{11} = 3$ state, but our analyses establish that nearly at the same frequency there is also the $J = 38 \leftarrow 37$ transition of the ($v_{10} = 1, v_{11} = 2$), $k = -1^+$ sublevel. According to the theoretical predictions from the present work (cf. Table 1), the latter lies ca. 290 cm⁻¹ below the $v_{10} = 3$ state and so a transition within the ($v_{10} = 1, v_{11} = 2$) combination tone is a more likely candidate for the observed feature. Finally, the present paper provides rather accurate theoretical predictions for term values of various low-lying bending vibrational states of HC₅N, which should be of help in determining the population distribution of vibrationally excited HC₅N in hot core sources and circumstellar shells.

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Table 4. Spectroscopic constants determined for the ($v_{10} = 1, v_{11} = 1$) and ($v_{10} = 1, v_{11} = 2$) bending combination states of HC₅N. Standard errors in units of the last digit are given in parentheses for the fitted parameters.

		($v_{10} = 1, v_{11} = 1$)	($v_{10} = 1, v_{11} = 2$)
<i>B</i>	(MHz)	1336.579275(24)	1339.381182(21)
<i>D</i>	(Hz)	32.3182(24)	33.8929(22)
<i>H</i>	(μHz)	1.635 ^a	1.635 ^a
<i>d_{JL(11,11)}</i>	(kHz)	-3.3047 ^a	-3.3316 ^a
<i>d_{JL(10,11)}</i>	(kHz)	3.467(44)	3.745(13)
<i>q₁₀</i>	(MHz)	0.50272(25)	0.50614(12)
<i>q_{10J}</i>	(Hz)	-0.1734 ^a	-0.197(12)
<i>q₁₁</i>	(MHz)	1.16704(34)	1.17182(13)
<i>q_{11J}</i>	(Hz)	-1.0629 ^a	-1.0714(60)
<i>q_{10,11,11}</i>	(kHz)		0.658(19)
<i>x_{L(11,11)}</i>	(GHz)		6.3053(14)
<i>x_{L(10,11)}</i>	(GHz)	7.3519(38)	7.34388(83)
<i>r_{10,11}</i>	(GHz)	-4.7974(52)	-4.7494(11)
<i>r_{10,11,J}</i>	(kHz)	-1.301(21)	-1.174(30)
<i>σ_{fit}</i>	(kHz)	10.1	10.6
No. of lines		84	130
<i>J</i> range		11–85	10–85

^a Fixed in the analysis.

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