Improved Molecular Constants of Acetylene 
Obtained from the $v_5$ Band System 

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A vibration-rotation band system of acetylene of the $J_1$ bending vibration $v_5$ has been recorded with high resolution by a Bruker IFS 120 HR Michelson spectrometer. From the analysis of the hot band of the normal isotopic species, $v_4 + v_5 - v_4$, and the fundamental band of HC$^{13}$CH in natural abundance an improved set of constants has been derived. The intensity perturbation due to the $l$-type resonance has been clearly observed in the band system $v_4 + v_5 - v_4$.

I. Introduction 

There exists a number of excellent spectroscopic papers concerning the vibration-rotation spectra of acetylene. Because of its large rotational constant, the spectra of this molecule were fairly well analyzed by Rao and coworkers [1], and Pliva and coworkers [2] using a large grating spectrometer. Recent improvement in the analysis was made by Hietanen and Kauppinen [3], who used their Michelson-type Fourier transform spectrometer.

In the present study we have remeasured the $v_5$ band of acetylene using the Gießen Fourier transform spectrometer in order to support our diode laser spectroscopic work near the 700 cm$^{-1}$ wave number region. In this frequency region the acetylene spectrum is rich and thus provides densely spaced calibration points. Several reasons stimulated the analysis of some bands in this spectrum resulting in an improved set of molecular constants: (i) the intrinsically beautiful and textbook like spectra warrant a closer investigation in their own right. As an example we compare in Fig. 1 the FT spectrum of the HC$^{13}$CH Q-branch near 728 cm$^{-1}$ with the cooled jet diode laser spectrum; (ii) recent supersonic jet spectroscopy shows that several interesting Van-der-Waals complexes can be formed with acetylene [4, 5] and (iii) acetylene is an interstellar molecule which is supposed to play an important role in the interstellar chemistry and can only be observed via its IR spectra [6].

This paper reports the spectrum and analysis of the hot band $v_4 + v_5 - v_4$ of the main species and of the $v_4$ band of HC$^{13}$CH. The high resolution Fourier transform spectrum supplies not only the usual large number of line positions but also gives fairly accurate line intensities of the transitions. In the present study we have used the latter FT property to discuss the intensity perturbation due to the $l$-type resonance.

II. Experimental Procedure and Observed Spectrum 

The spectrum was recorded with a Bruker IFS 120 HR vacuum Michelson-type interferometer in Gießen [7]. Using a 17 cm long cell we have measured the spectrum at a pressure of about 85 Pa at room temperature and with a resolution of 0.0036 cm$^{-1}$. The line positions were calibrated by using CO$_2$ lines as the wavenumber standard [8]. The recording of the spectrum spans from 410 to 970 cm$^{-1}$; we covered such a large frequency region in order to use the spectrum to calibrate our diode laser spectrometers. In the present paper we report only on the analysis of a small portion of the observed spectrum. One Q-branch structure is reproduced in Fig. 2 to demonstrate the quality of the spectrum. Industry grade acetylene was used as the sample gas without further purification.

Although the $B$ rotational constant of this molecule is very large, about 35 GHz, the observed absorption lines are fairly densely populated due to the excitation...
Fig. 1. Comparison of FT and cooled jet diode laser spectrum of the HC\(^{13}\)CH (0, \(^1\)–(0, 0) Q-branch. As expected, no intensity alternation is observed for adjacent \(J\)-lines.

Fig. 2. A portion of the observed spectrum showing the Q-branch region of the \((1, 1)^2–(1, 0)^1\) band near 731.1 cm\(^{-1}\). The spectrum of the symmetric species shows the 3 : 1 intensity alternation caused by the hydrogen nuclear spin.
of many hot and isotope bands. Among them we have analyzed the hot band from the $I_a$ bending vibration $v_4=1$ state, i.e. the hot band $v_4+v_5-v_4$, because the $I_a$ bending vibration is infrared inactive and this band is one of the limited sources of information of the $v_4=1$ state. In addition we have analyzed the $v_5$ band of HC$^{13}$CH. We apply the numbering of the normal modes of the symmetric species for this asymmetrical molecule as well, although the center of symmetry is missing as a means to distinguish $n$ molecule as well, although the center of symmetry is $\pi$ state, i.e. the hot band $v_4$, because the $t; l$ indicates -1- or $l$ indicates $+$ or $-$ in Wang’s combination. The corresponding wavefunctions are given by $|v_4, v_5; l t\rangle$. These notations are the same as used for HCCCCN and DCCCCN by Yamada and coworkers [10, 11]. We repeat here the most important definitions: Wang’s linear combinations used in the present study are

$$|0, 1; 1^\pm\rangle = \{|0^0, 1^1; J, 1\rangle \pm |0^1, 1^1; J, 1\rangle\}/\sqrt{2},$$

$$|1, 0; 1^\pm\rangle = \{|1^0, 1^1; J, 1\rangle \pm |1^1, 1^1; J, 1\rangle\}/\sqrt{2},$$

$$|1, 1; 0^\pm\rangle = \{|1^1, 1^1; J, 0\rangle \pm |1^1, 1^1; J, 0\rangle\}/\sqrt{2},$$

$$|1, 1; 2^\pm\rangle = \{|1^1, 1^1; J, 2\rangle \pm |1^1, 1^1; J, 2\rangle\}/\sqrt{2},$$

where the basis function $|v_4^l, v_5^l; J, l\rangle$ is the product of the wavefunctions of the two-dimensional-isotropic oscillators and the symmetric top wavefunction. The phases of the basis wavefunctions are so chosen that

$$\varrho = \delta_4 = \delta_5 = 0$$

in the sense of Yamada [12].

### The (0, 0) Band of HC$^{13}$CH

There are well known problems for the sign of the off-diagonal matrix elements of the linear-molecule Hamiltonian. However in the present case the sign of the $q_5$ constant has been uniquely determined, since we have observed also the well resolved Q-branch transitions in addition to those of the P and R branches. The selection rule for the Q-branch of the $(0, 1)-(0, 0)$ band is $f-e$, and for the P and R branches $e-e$. Thus we were able to determine the symmetry and the energy of both of the l-doubling components in the $(0, 1)$ state simultaneously. The analysis of the present data leads to a unique conclusion of positive $q_5$.

The constants obtained by the least-squares analysis are listed in Table 1. The observed transition wave numbers are listed in Table 2.
Table 1. Spectroscopic parameters of HC¹³CH obtained in the present study*.

<table>
<thead>
<tr>
<th>Constant</th>
<th>Ground state</th>
<th>(v_s = 1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(G_s/\text{cm}^{-1})</td>
<td>(729.378362(67))</td>
<td></td>
</tr>
<tr>
<td>(B_s/\text{MHz})</td>
<td>(34429.954(67))</td>
<td></td>
</tr>
<tr>
<td>(D_s/\text{kHz})</td>
<td>(46.646(48))</td>
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</tr>
<tr>
<td>(H_p/\text{Hz})</td>
<td>(-0.027(33))</td>
<td></td>
</tr>
<tr>
<td>(q_d/\text{MHz})</td>
<td>(134.386(13))</td>
<td></td>
</tr>
<tr>
<td>(q_s/\text{kHz})</td>
<td>(-1.090(15))</td>
<td></td>
</tr>
</tbody>
</table>

* Numbers in parentheses are uncertainties in one standard deviation in units of the last digit quoted.

The (1, 1) – (1, 0) Band of HCCH

The signs of the off-diagonal constants should be handled carefully in this case. Since the normal species has a center of symmetry, the intensity alternation due to the spin statistics supplies unambiguous information for the symmetry of the energy levels as listed in Table 3. The symmetry combined with the transition frequencies allowed only one choice for the signs of \(q_4\) of the (1, 0) state and \(r_{45}\) of the (1, 1) state: positive \(q_4\) and negative \(r_{45}\). From the transition frequencies the signs of the constants \(q_4\) and \(q_5\) of the (1, 1) state are determined with the assumption that the constants do not change much for the various vibrational states.

As we can see from the energy matrix of the (1, 1) state in the symmetrized basis, which is by neglecting the higher order off-diagonal terms

\[
\begin{pmatrix}
| (1, 1)^0 \rangle > | (1, 1)^2 \rangle > | (1, 1)^0 \rangle > | (1, 1)^2 \rangle > | (1, 1)^0 \rangle > | (1, 1)^2 \rangle > | (1, 1)^0 \rangle > | (1, 1)^2 \rangle > | (1, 1)^0 \rangle > & | (1, 1)^2 \rangle > | (1, 1)^0 \rangle > | (1, 1)^0 \rangle > | (1, 1)^2 \rangle > | (1, 1)^0 \rangle > | (1, 1)^2 \rangle > | (1, 1)^0 \rangle > | (1, 1)^2 \rangle > | (1, 1)^0 \rangle > | (1, 1)^2 \rangle > \\
\end{pmatrix}
\]

where \(E_{ij}\) are the matrix elements of the diagonal operator \(\hat{h}_q\) and

\[f = (1/2) \sqrt{J(J+1)[J(J+1)-2]},\]

we can determine the absolute values of the sum and difference of the two \(l\)-type doubling constants from the energy analysis. However, as discussed by Di Lauro and Mills [13] for the Coriolis interaction, we can also determine the signs of the off-diagonal matrix elements from the intensity analysis. The sign information is carried by the eigenfunction and is revealed in the line intensity.

Table 2. Observed line positions of HC¹³CH in the \(v_s\) band in cm⁻¹.

<table>
<thead>
<tr>
<th>(J)</th>
<th>(P)</th>
<th>(Q)</th>
<th>(R)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\text{observed})</td>
<td>(\text{obs.- calc.})</td>
<td>(\text{obs.- calc.})</td>
<td>(\text{obs.- calc.})</td>
</tr>
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<td>735.11575</td>
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<td>33</td>
<td>728.23669</td>
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<td>735.11575</td>
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Table 3. Symmetry and nuclear spin statistics.

<table>
<thead>
<tr>
<th>(J) even</th>
<th>(q_4)</th>
<th>(J) odd</th>
<th>(q_4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\Sigma_{ul}^+)</td>
<td>(1, 1)^0\rangle e + a 3</td>
<td>-s 1</td>
<td>3</td>
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<tr>
<td>(\Sigma_{ul}^-)</td>
<td>(1, 1)^2\rangle f - s 1</td>
<td>+ a 3</td>
<td>6</td>
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<td>(\Lambda_{ul}^+)</td>
<td>(1, 1)^0\rangle e + a 3</td>
<td>-s 1</td>
<td>3</td>
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<tr>
<td>(\Lambda_{ul}^-)</td>
<td>(1, 1)^2\rangle f - s 1</td>
<td>+ a 3</td>
<td>6</td>
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</tbody>
</table>

Figure 3 shows the Boltzmann plot for the observed transitions using the correct perturbed wavefunctions compared with that using unperturbed wavefunctions and that using wavefunctions calculated with improper signs of \(q_4\) and \(q_5\). The Boltzmann plot is a diagram showing the energy dependence of the
Fig. 3. Boltzmann-plot for P- and R-transitions to (upper) substates / = 0 and / = 2 using (A) the unperturbed wavefunction, (B) an incorrect wavefunction (qA and qB negative), and (C) the true wavefunction.

Table 4. Spectroscopic parameters of HCCH obtained in the present study.

<table>
<thead>
<tr>
<th>Constant</th>
<th>(v4, v3) = (1, 0)</th>
<th>(v4, v3) = (1, 1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>G/cm⁻¹</td>
<td>612.871</td>
<td>1 340.916082(29)</td>
</tr>
<tr>
<td>B/μHz</td>
<td>198 006.1(10)</td>
<td>35 383.795(34)</td>
</tr>
<tr>
<td>dJ/μHz</td>
<td>35.133.548(32)</td>
<td>-3.3906(47)</td>
</tr>
<tr>
<td>D4/kHz</td>
<td>49.641 (23)</td>
<td>50.372 (22)</td>
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<tr>
<td>qA/μHz</td>
<td>156.827 (13)</td>
<td>159.72 (11)</td>
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<tr>
<td>qB/μHz</td>
<td>-1.213 (35)</td>
<td>-1.280 (66)</td>
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<tr>
<td>qv/μHz</td>
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<tr>
<td>q3/μHz</td>
<td>143.377 (55)</td>
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<td>q5/μHz</td>
<td>-1.131 (39)</td>
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<td>r4/μHz</td>
<td>-187.033.3 (13)</td>
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<td>r5/μHz</td>
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<tr>
<td>r6/μHz</td>
<td>-0.1458 (77)</td>
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* Numbers in parentheses are uncertainties in one standard deviation in units of the last digit quoted.


logarithm of the population obtained from the observed line intensities and the calculated line strength. If the line strengths based on the wavefunctions of the lower and upper states are correct, and if the distribution is boltzmannian, the diagram shows a single straight line, the slope of which is proportional to (kT)⁻¹, where T is the thermodynamical temperature of the sample during measurement. Figure 3 (A) shows that the J-dependent intensity anomalies are not taken care of by the normal Hönl-London type intensity expression: the temperature obtained from the 2⁺−1⁻ band is apparently lower than that from the 0⁺−1⁻ band. This effect is caused by the reduction of the intensity of the former band and enhancement of}

Table 5. Observed line positions of HCCH in the v4 + v5 − v4 band in cm⁻¹; transitions from l = 1 to l = 0 substate.*

<table>
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<tr>
<th>J</th>
<th>P</th>
<th>Q</th>
<th>R</th>
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<td>32</td>
<td>653.01880</td>
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<td>810.55679</td>
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</table>

* In this table and following tables, parity of upper state is determined by the selection rules: e-e and f-f for P- and R-branches and e-f for Q-branches.
the latter by the mixing of the wavefunctions due to the l-type resonance. If we correct this effect, we obtain Fig. 3 (C): both bands show a consistent temperature. If we use incorrect sign of the q's, the inconsistence in the temperature increases: this is shown in Figure 3(B).

By using the Boltzmann plot for all possible choices we have determined uniquely the value (including its sign) of \( q_a \) and \( q_b \) in the (1, 1) vibrational states. The constants thus determined by a least-squares analysis are listed in Table 4. The measured transitions are contained in Tables 5–8.

### IV. Conclusion

We report here improved spectroscopic constants of HC\(^{13}\)CH in the ground and \( v_9 = 1 \) states, and those of HCCCH in the \( v_4 = 1 \) and \( (v_4, v_9) = (1, 1) \) states. The present results are consistent with values quoted in the literature, especially they are in a good agreement with Hietanen and Kauppinen [3]. The present work has been carried out with slightly better resolution and consequently better precision.

The line intensities also supply important information about the molecular constants. In the present
Table 8. Observed line positions of HCCH in the \( v_4 + v_5 - v_4 \) band in cm\(^{-1}\): transitions from \( l=1^- \) to \( l=2 \) substate.

<table>
<thead>
<tr>
<th>( J )</th>
<th>( P )</th>
<th>( Q )</th>
<th>( R )</th>
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study it is shown that one can determine the sign of the \( \ell \)-type resonance interaction constants by using the intensity anomaly. In the other words, we have found that the \( \ell \)-type resonance interaction produces an unignorable amount of intensity change. Since this resonance is a common interaction for linear molecules, i.e. an inherent interaction and not accidental, we would like to stress that the \( \ell \)-type resonance effect has to be always taken into account in the intensity analysis of a linear molecule.

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